Supporting information

Chemoselective [3+2] annulation of oxime acetate with 2-aryl-3-ethoxycarbonyl-pyrroline-4,5-dione: Entry to pyrrolo[2,3-*b*] pyrrole derivatives

Andhavaram Ramaraju,[a,b] Atul Upare,[a] Ewan W. Blanch,[b] Subashani Maniam,[b] Balasubramanian Sridhar,[c] Surendar Reddy Bathula[a,d] and Chada Raji Reddy,*[,a]

[a]Department of Organic Synthesis & Process Chemistry, CSIR-Indian Institute of Chemical Technology, Hyderabad - 500007, India,
[b]School of Science, STEM College, RMIT University, Melbourne, Victoria, 3001, Australia.
[c]*Center for X-ray Crystallography, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, India.*
[d]*Deceased on 30th August, 2020.*

E-mail: rajireddy@iict.res.in

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1. Single X-ray crystal data of compound 3m:

X-ray data for the compounds were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073Å) with ω-scan method [1]. Preliminary lattice parameters and orientation matrices were obtained from four sets of frames.

Integration and scaling of intensity data were accomplished using SAINT program [1]. The structure was solved by direct methods using SHELXS [2] and refinement was carried out by full-matrix least-squares technique using SHELXL [2]. Anisotropic displacement parameters were included for all non-hydrogen atoms. The N-bound H atom was located in difference Fourier maps and their positions and isotropic displacement parameters were located and refined. All other H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å and U_{iso}(H) = 1.2U_{eq}(c) for H atoms]. The atoms C16, C20 and C21 were disordered over two sites and their site occupation factors were refined to 0.677(7) and 0.323(7), respectively. Equal anisotropic displacement parameters (EADP) and distance constraints (DFIX) were applied for the disordered groups.

Crystal structure determination of 3m

Crystal Data for $C_{21}H_{17}N_2O_4Cl$ (*M* =396.82 g/mol): monoclinic, space group C2/c (no. 15), *a* = 27.3068(11) Å, *b* = 7.9003(3) Å, *c* = 18.7137(8) Å, *β* = 108.0280(10)°, *V* = 3838.9(3) Å^3, *Z* = 8, *T* = 294.15 K, μ(MoKα) = 0.229 mm^{-1}, *Dcalc* = 1.373 g/cm^3, 18454 reflections measured (4.578° ≤ 2Θ ≤ 49.998°), 3396 unique (R_{int} = 0.0236, R_{sigma} = 0.0173) which were used in all calculations. The final R_1 was 0.0808 (I > 2σ(I)) and wR_2 was 0.2161 (all data). CCDC 1967145 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

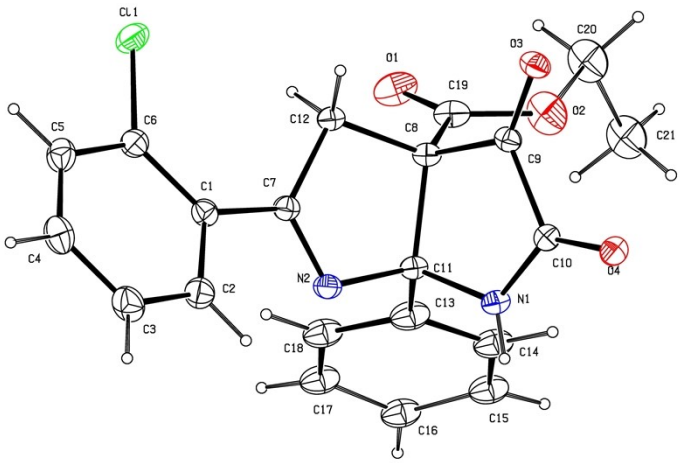
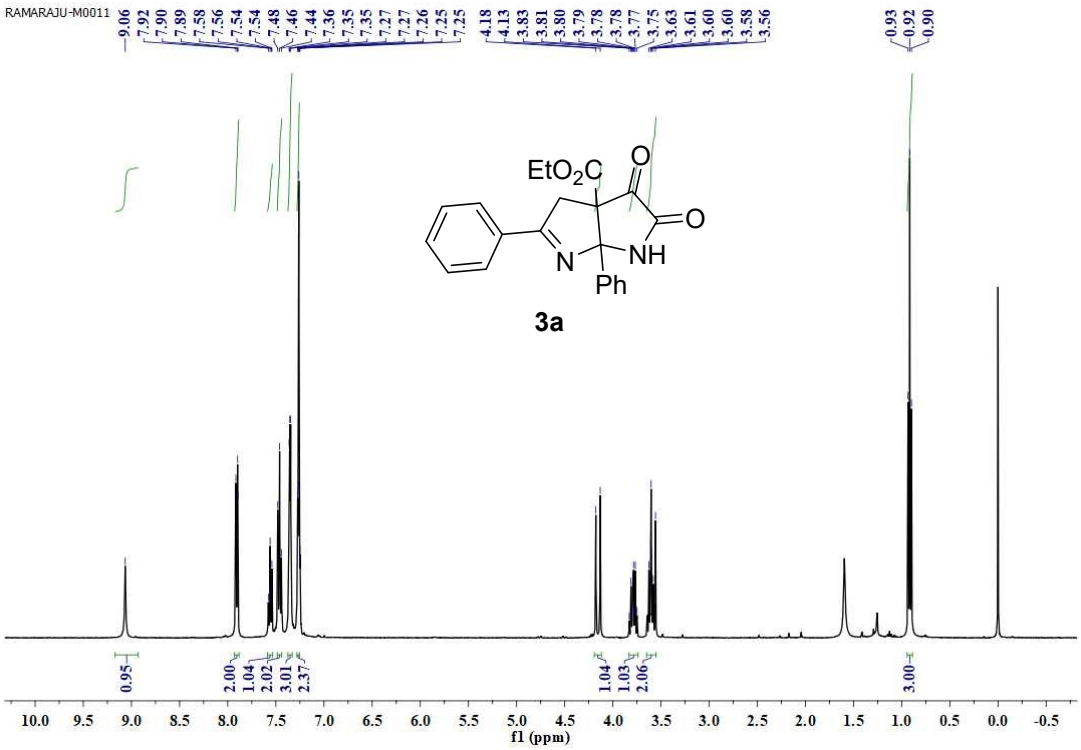


Fig.1.A view of **3m**, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii. The minor disordered components were omitted for clarity.

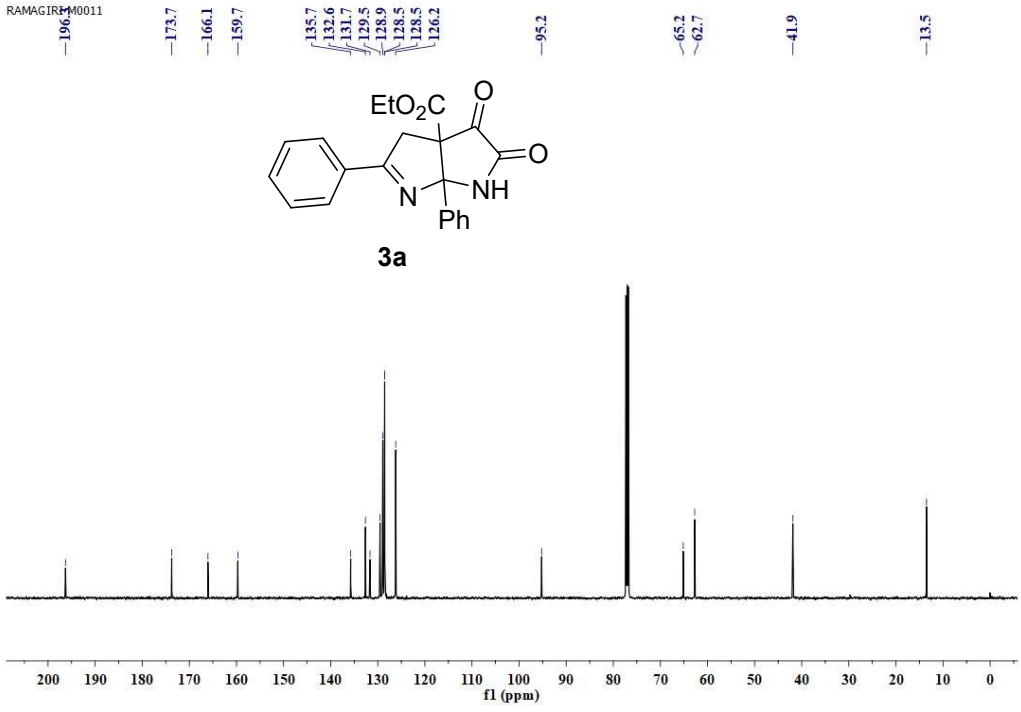
[1] Bruker (2001). SAINT (Version 6.28a) & SMART (Version 5.625). Bruker AXS Inc., Madison, Wisconsin, USA.

[2] Sheldrick G. M. (2015**)** Acta Crystallogr C71: 3-8.

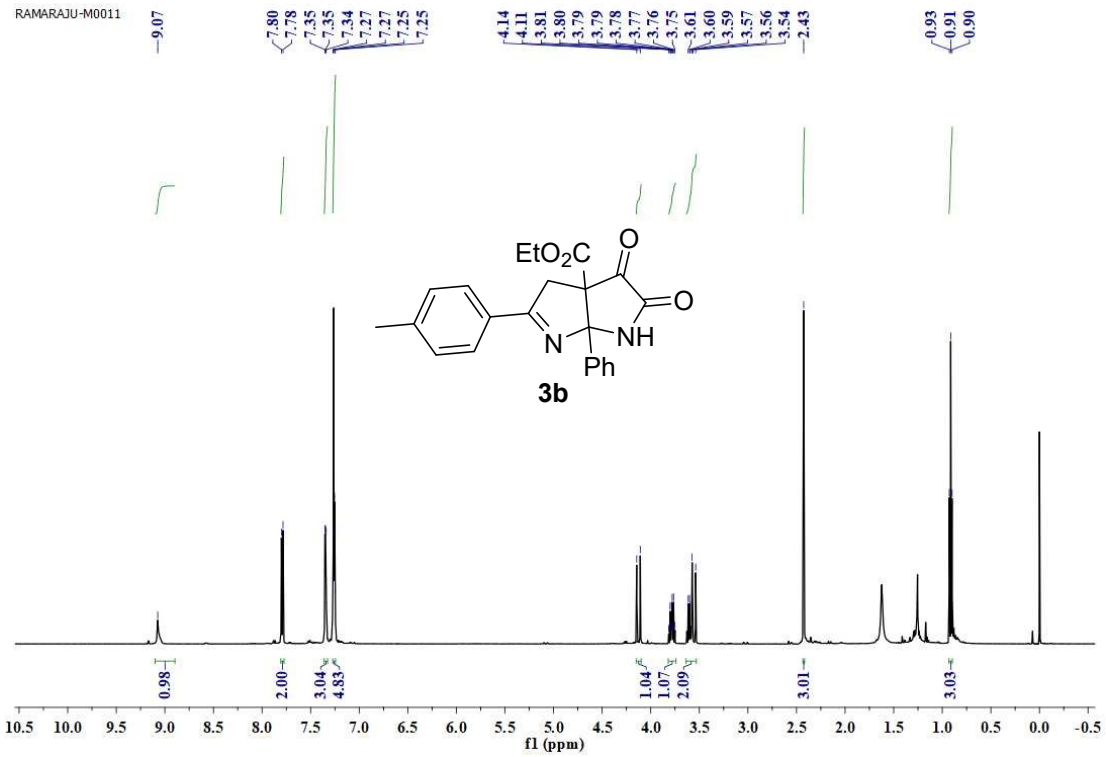
2. ^{1}H and ^{13}C NMR spectra:



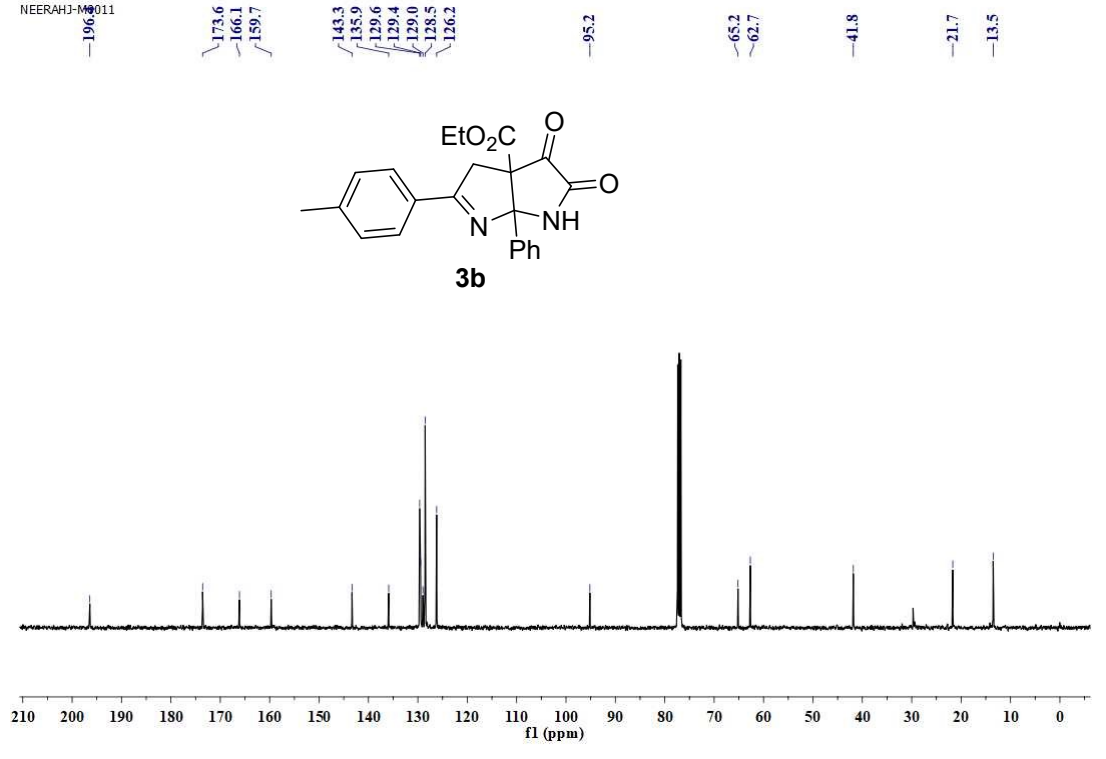
^{1}H-NMR spectrum of **3a** (400 MHz, $CDCl_3$)



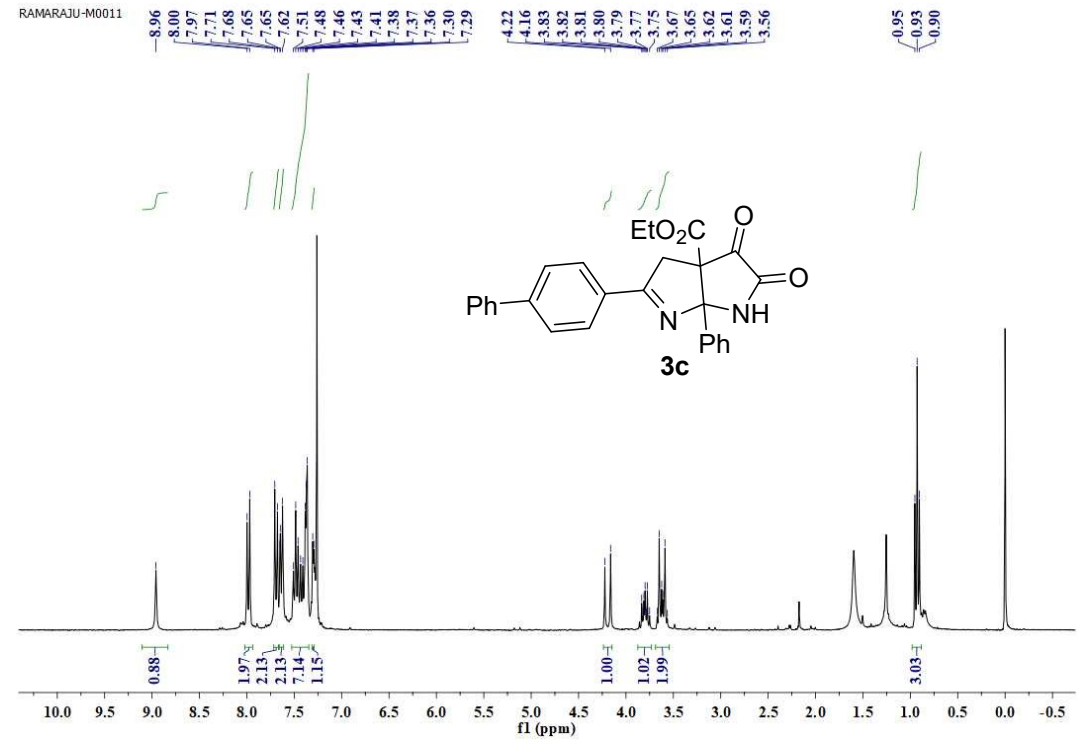
^{13}C-NMR spectrum of **3a** (125 MHz, $CDCl_3$)



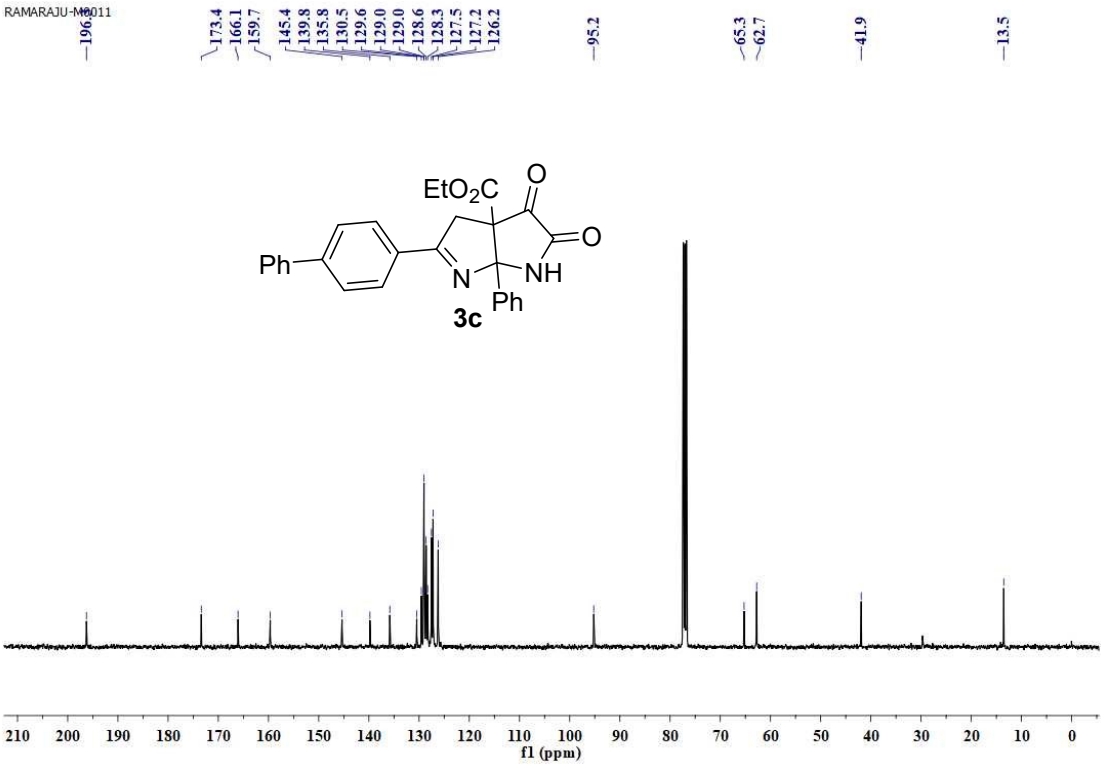
^{1}H-NMR spectrum of **3b** (500 MHz, $CDCl_3$)



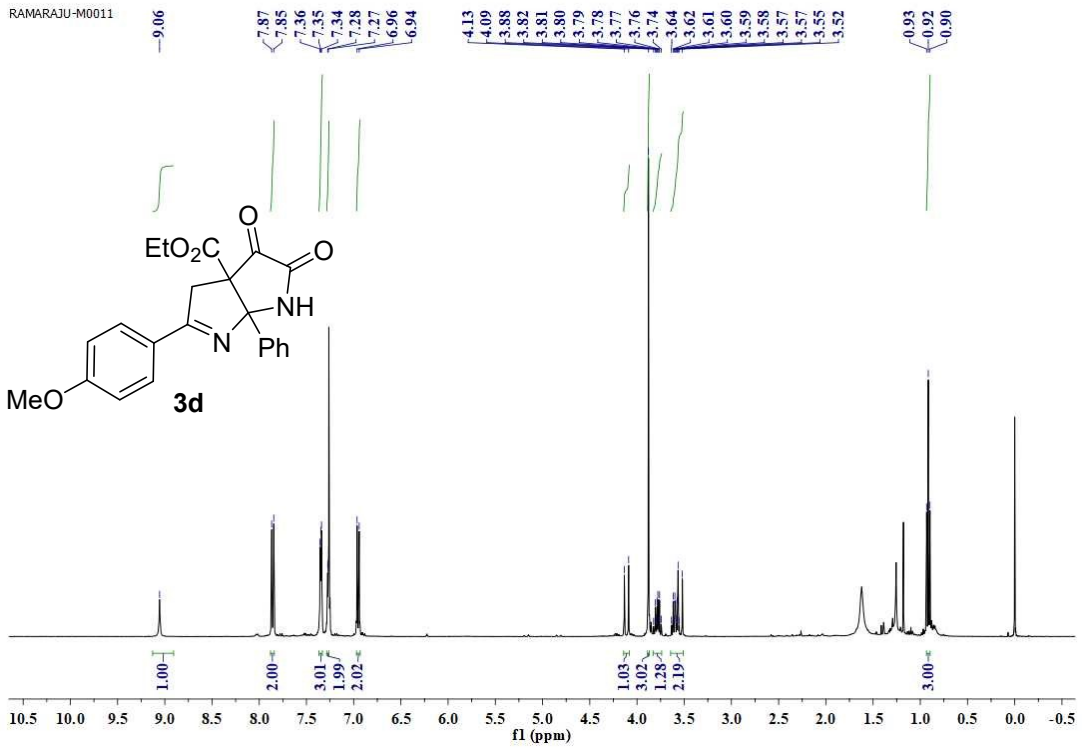
^{13}C-NMR spectrum of **3b** (100 MHz, $CDCl_3$)



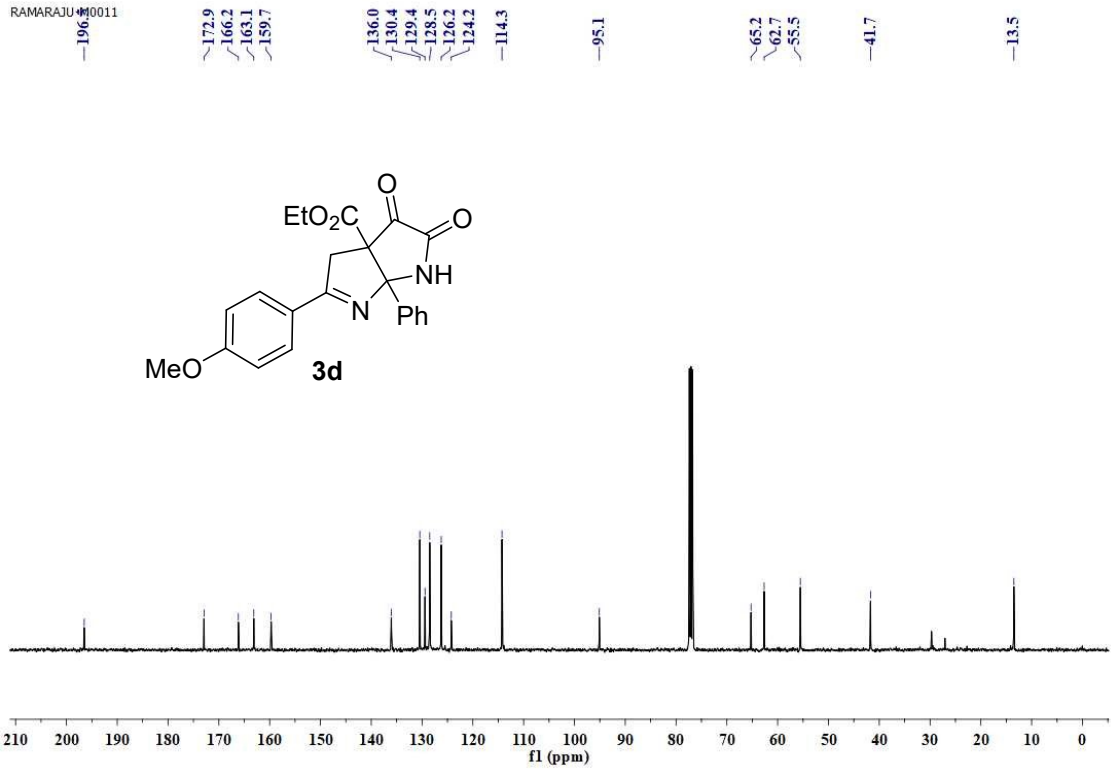
^{1}H-NMR spectrum of **3c** (300 MHz, $CDCl_3$)



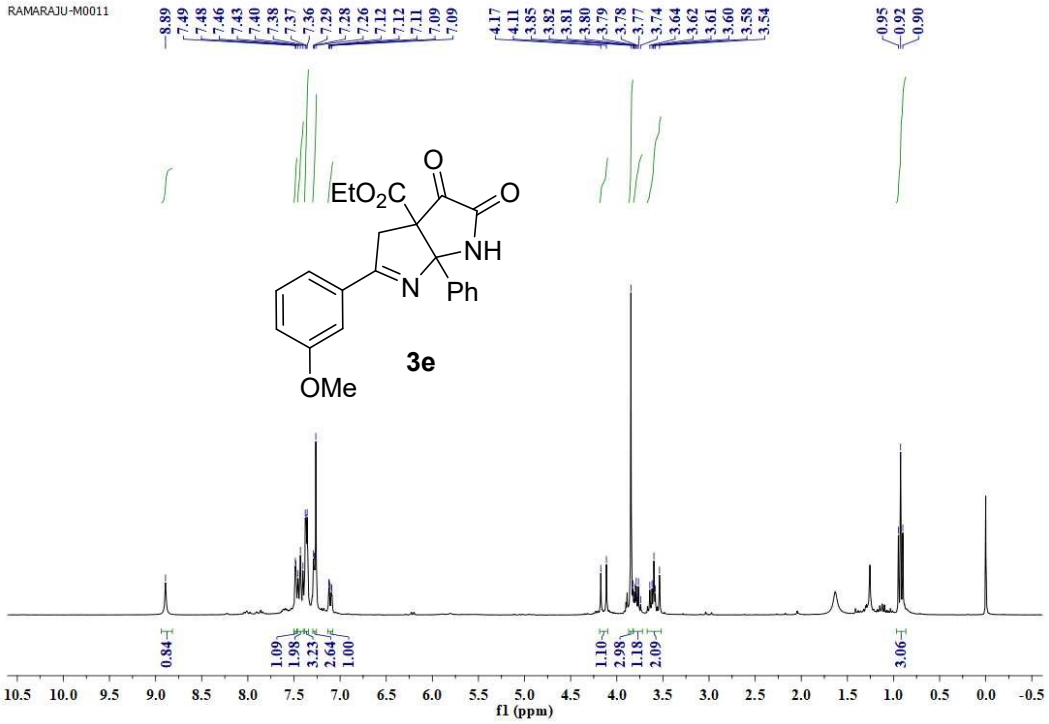
^{13}C-NMR spectrum of **3c** (100 MHz, $CDCl_3$)



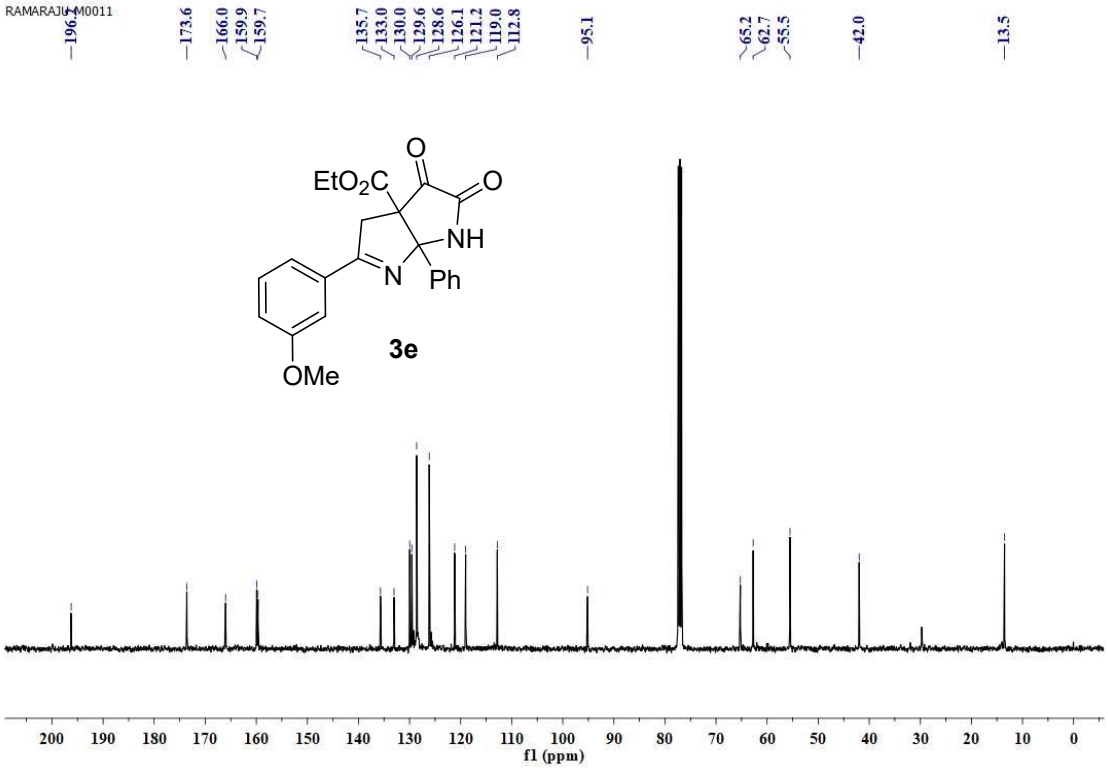
^{1}H-NMR spectrum of **3d** (400 MHz, $CDCl_3$)



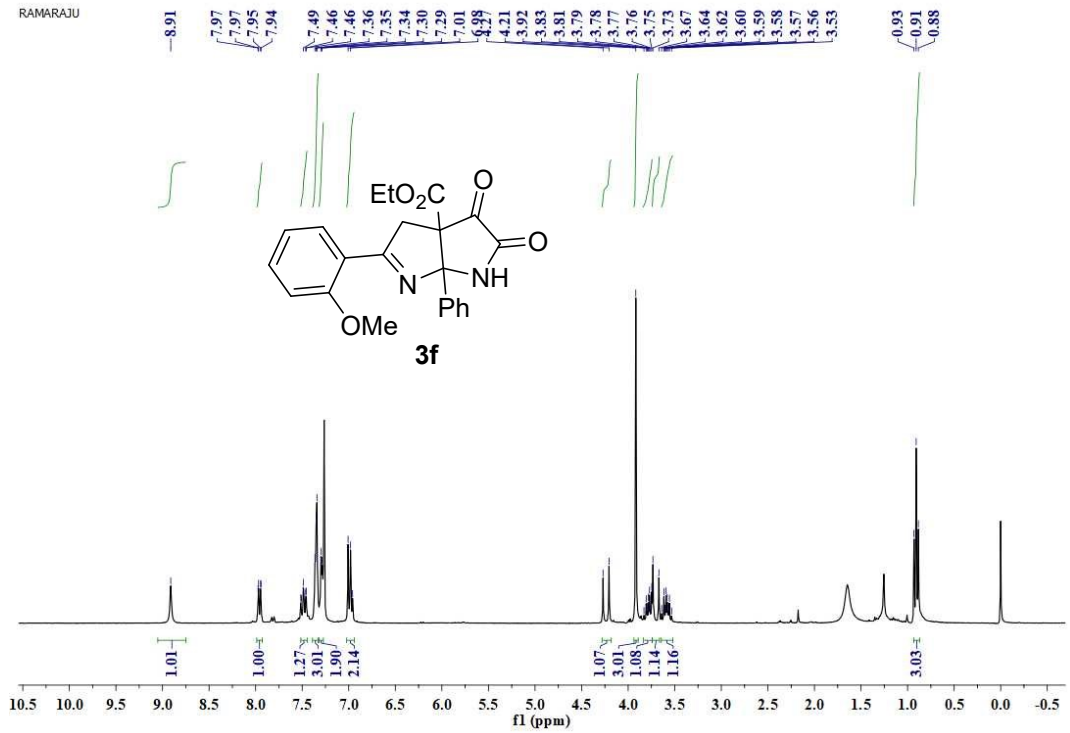
^{13}C-NMR spectrum of **3d** (100 MHz, $CDCl_3$)



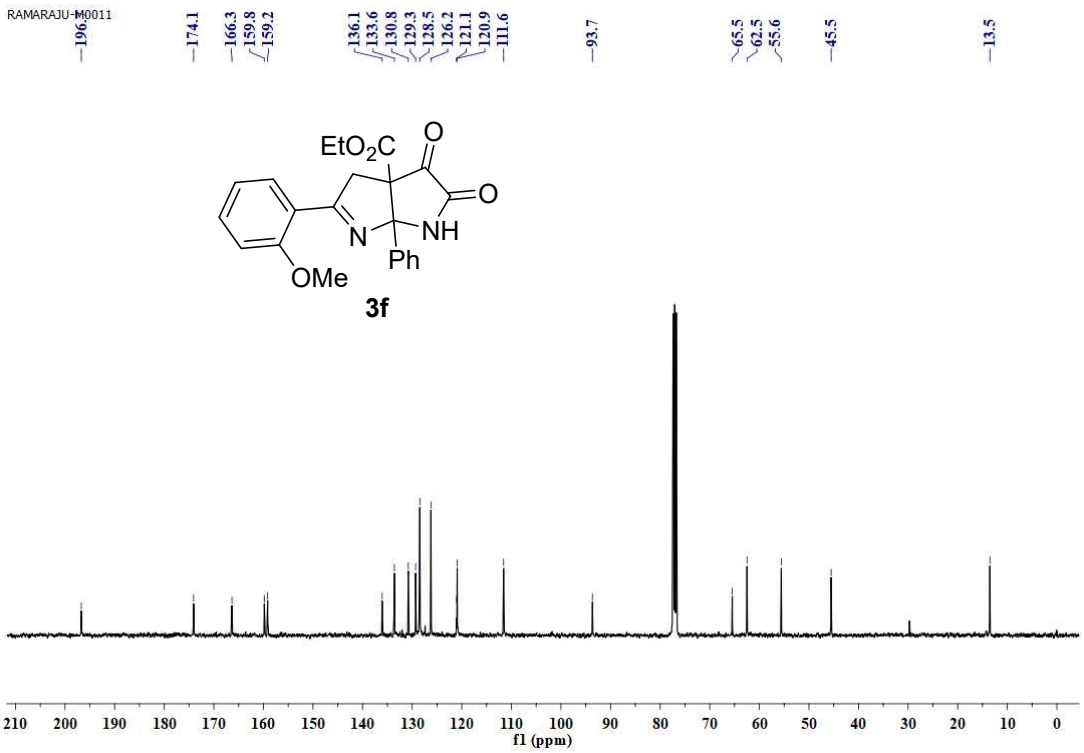
^{1}H-NMR spectrum of **3e** (300 MHz, $CDCl_3$)



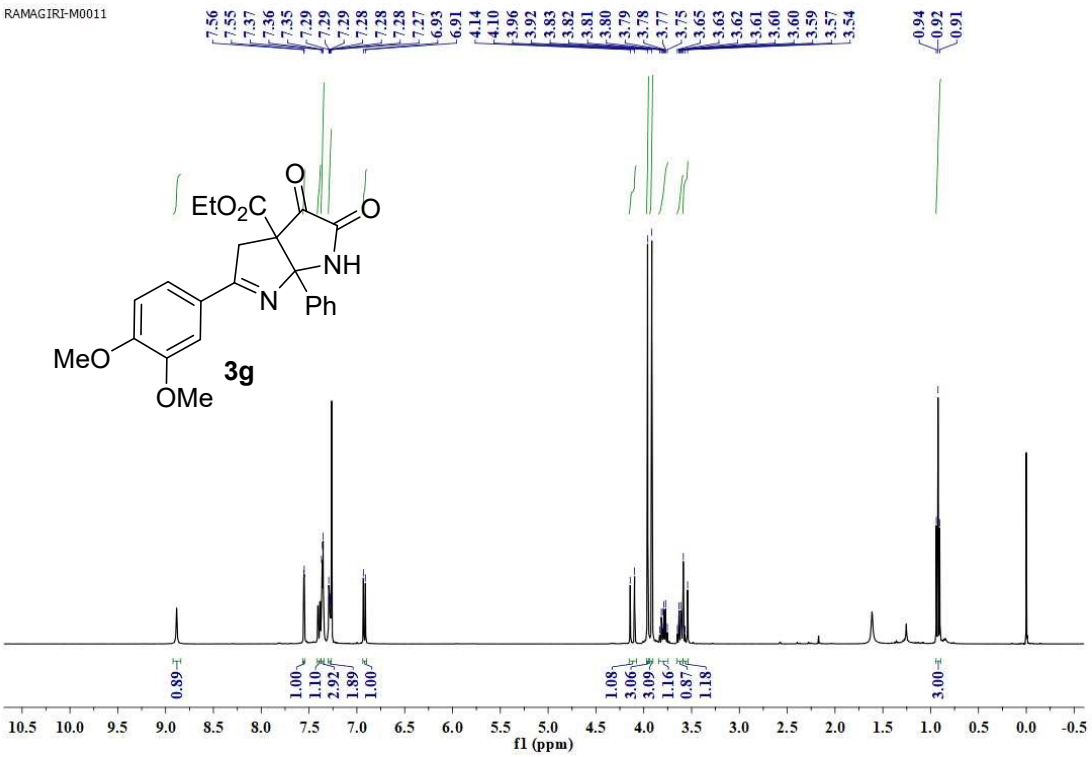
^{13}C-NMR spectrum of **3e** (100 MHz, $CDCl_3$)



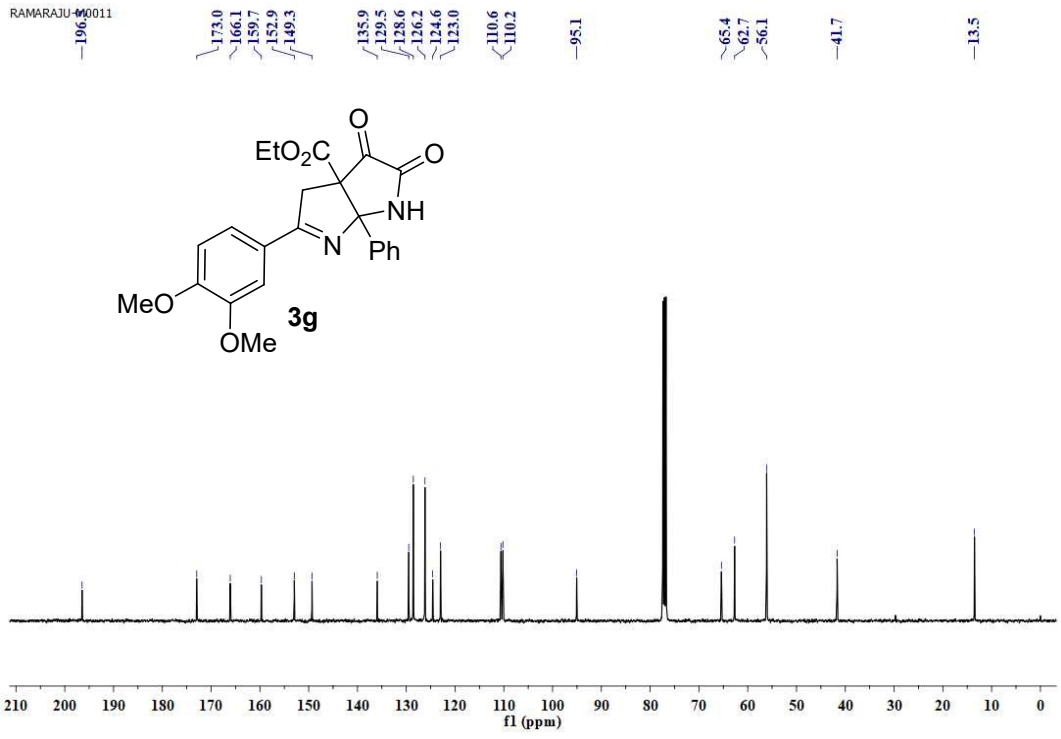
^{1}H-NMR spectrum of **3f** (300 MHz, $CDCl_3$)



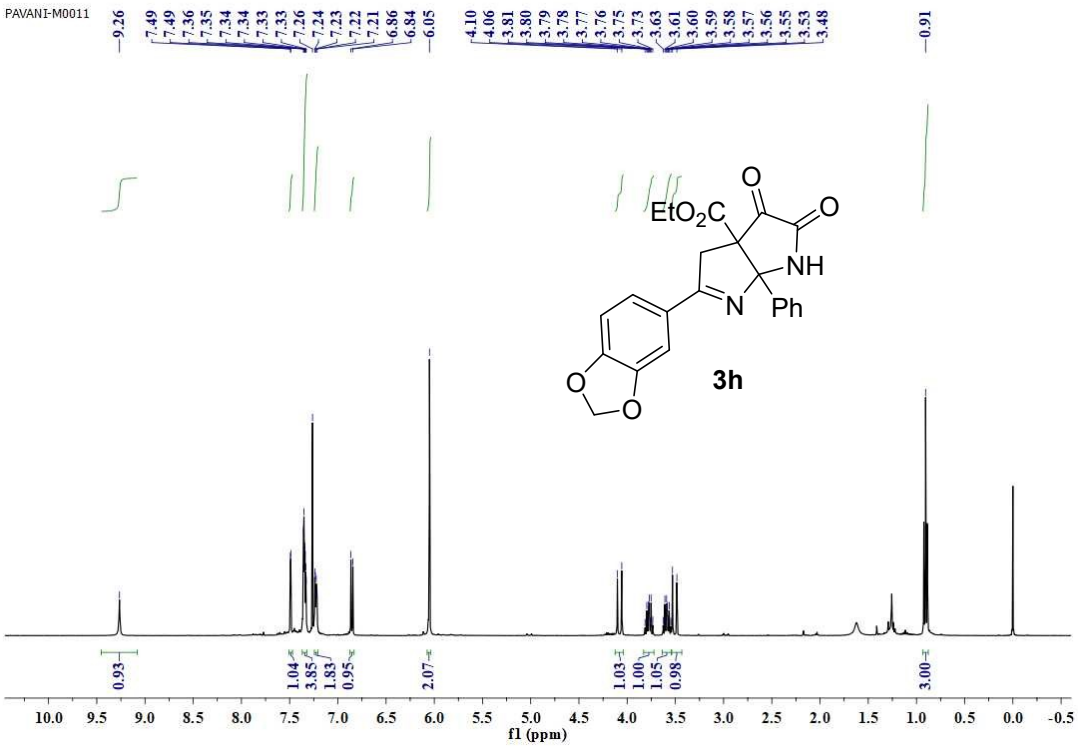
^{13}C-NMR spectrum of **3f** (100 MHz, $CDCl_3$)



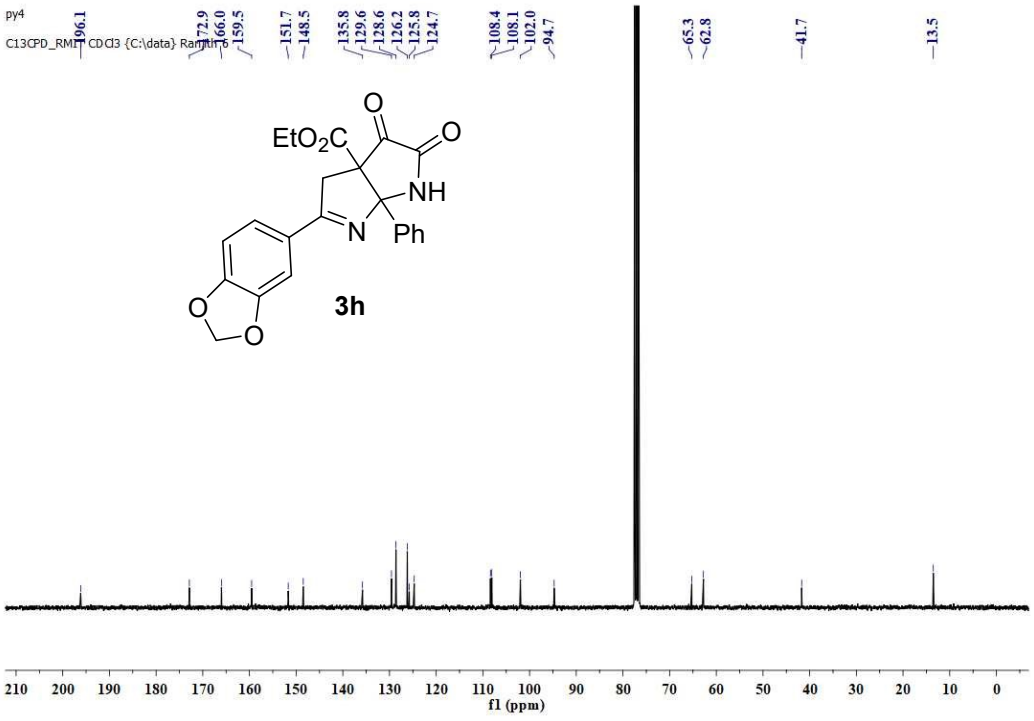
^{1}H-NMR spectrum of **3g** (400 MHz, $CDCl_3$)



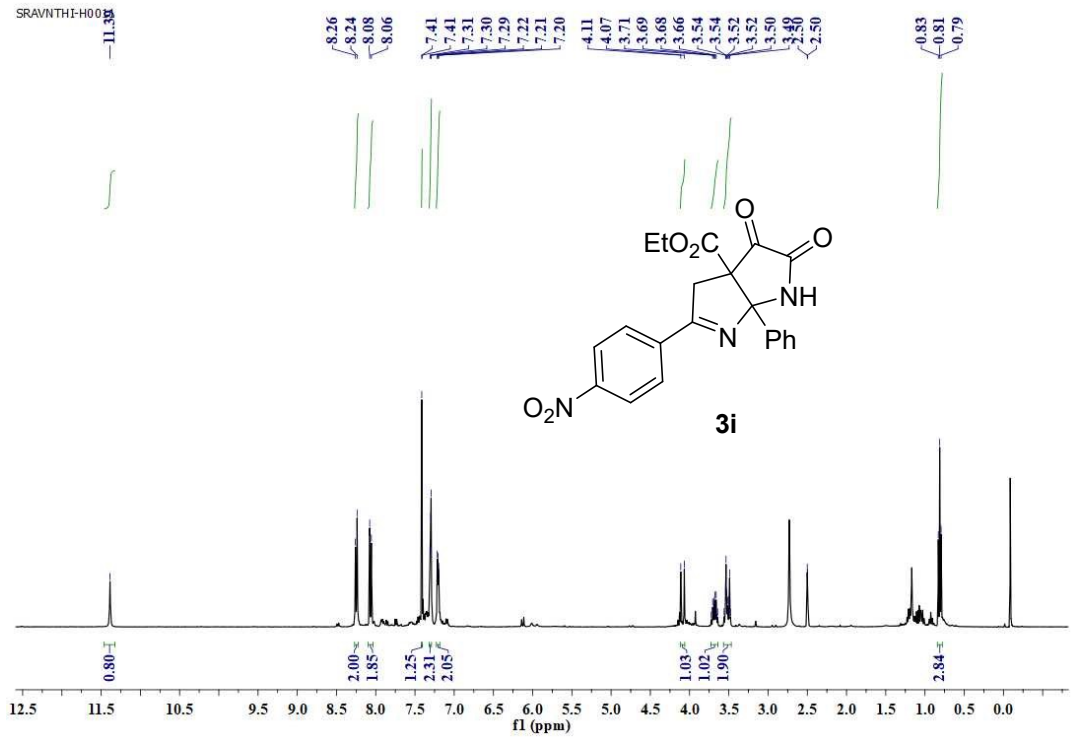
^{13}C-NMR spectrum of **3g** (100 MHz, $CDCl_3$)



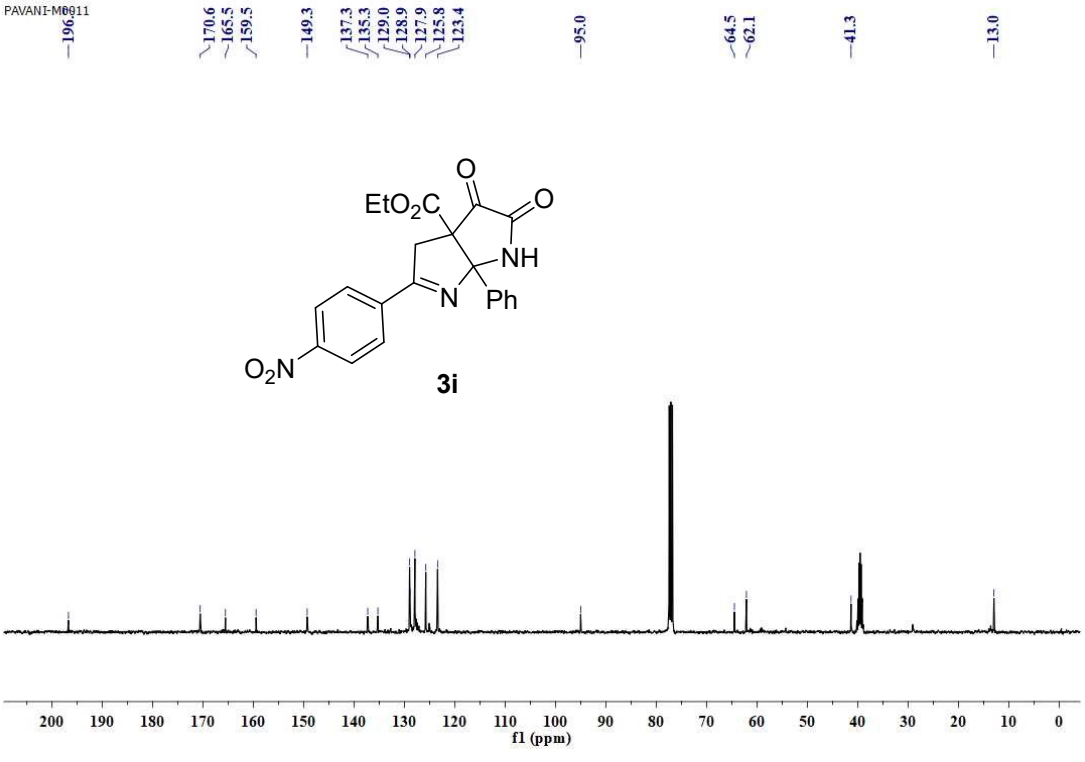
^{1}H-NMR spectrum of **3h** (400 MHz, $CDCl_3$)



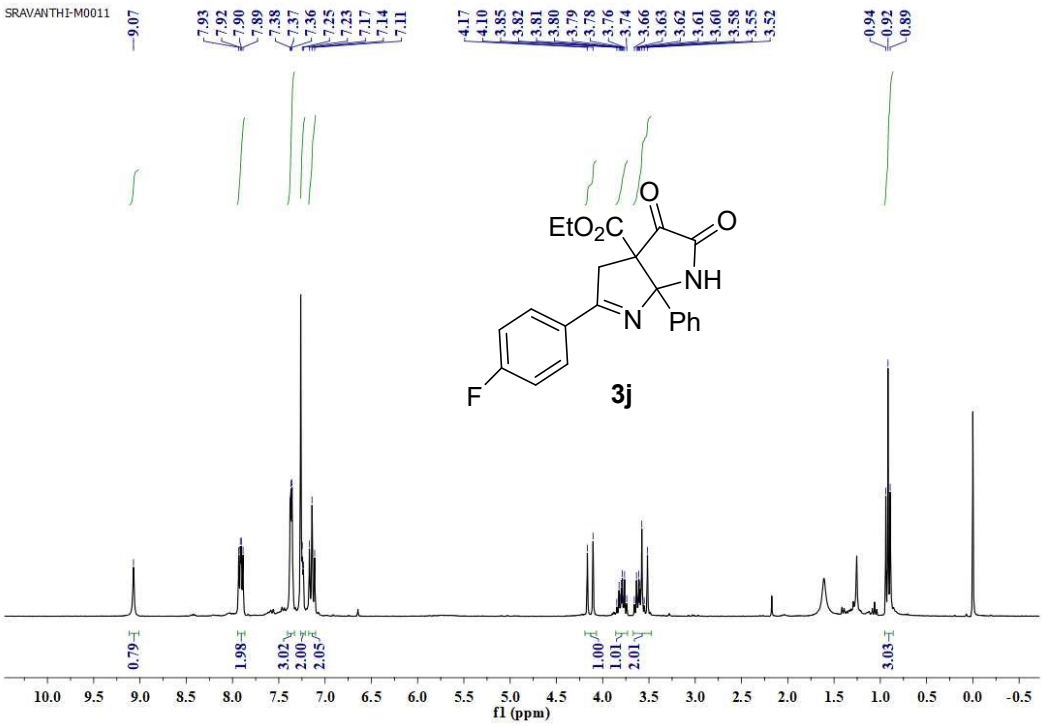
^{13}C-NMR spectrum of 3**h** (75 MHz, $CDCl_3$)



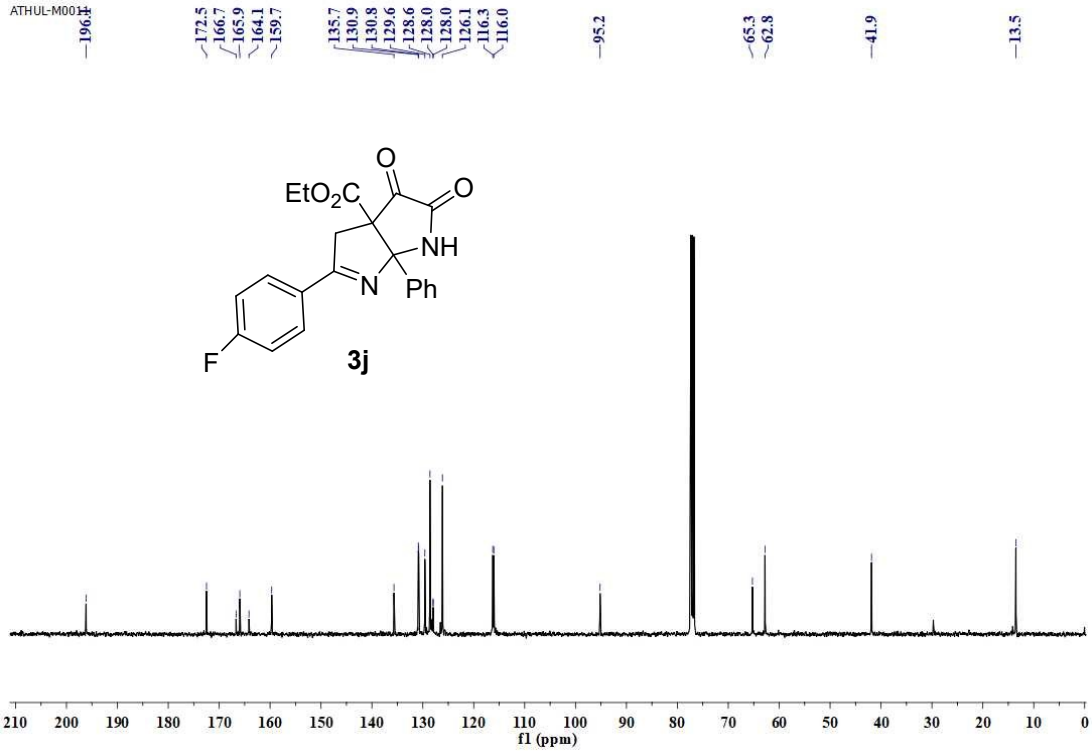
^{1}H-NMR spectrum of **3i** (400 MHz, $CDCl_3$ +DMSO-d_6)



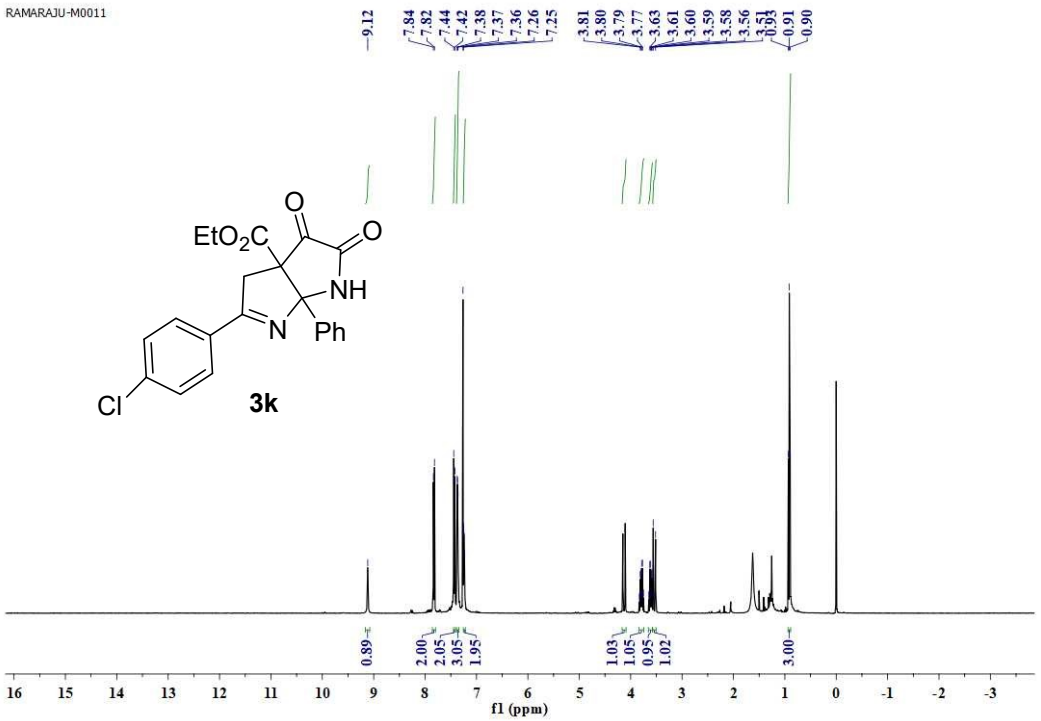
^{13}C-NMR spectrum of 3i (100 MHz, $CDCl_3$)



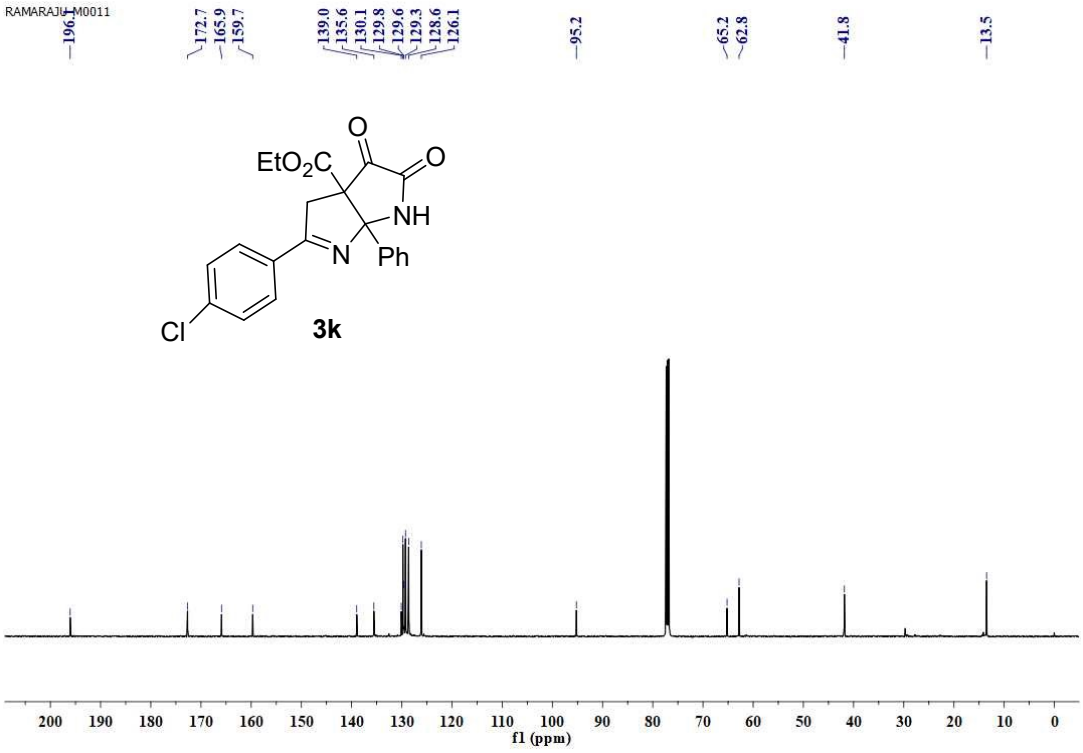
^{1}H-NMR spectrum of **3j** (300 MHz, $CDCl_3$)



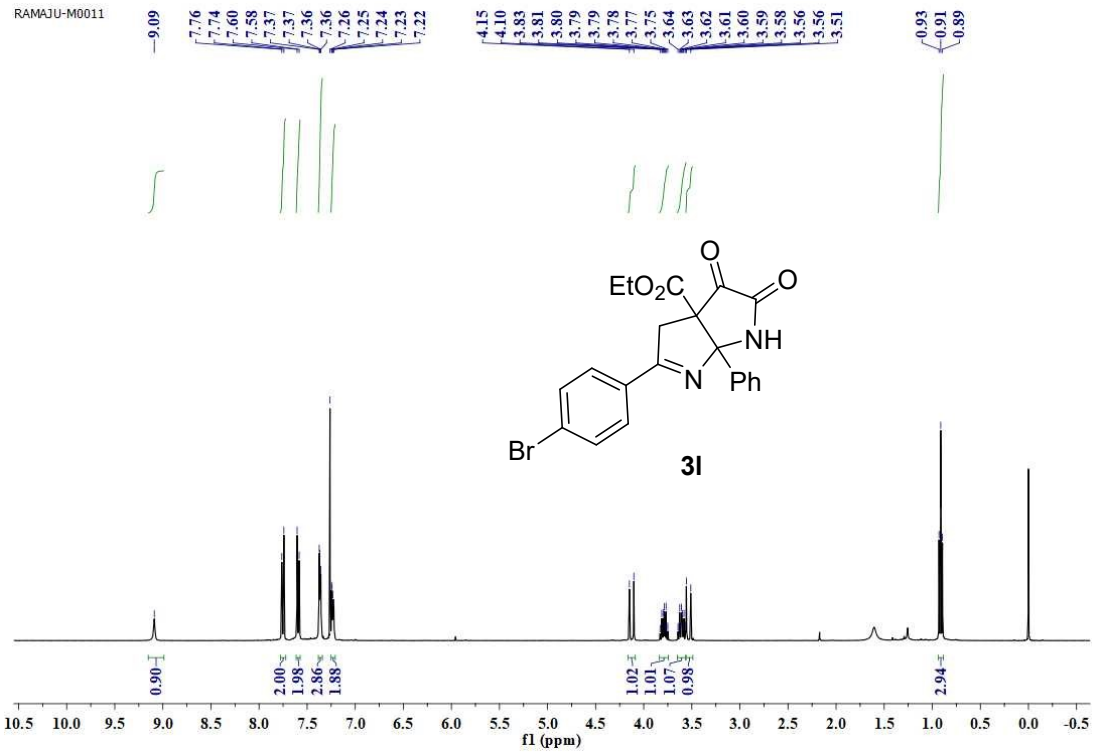
^{13}C-NMR spectrum of **3j** (100 MHz, $CDCl_3$)



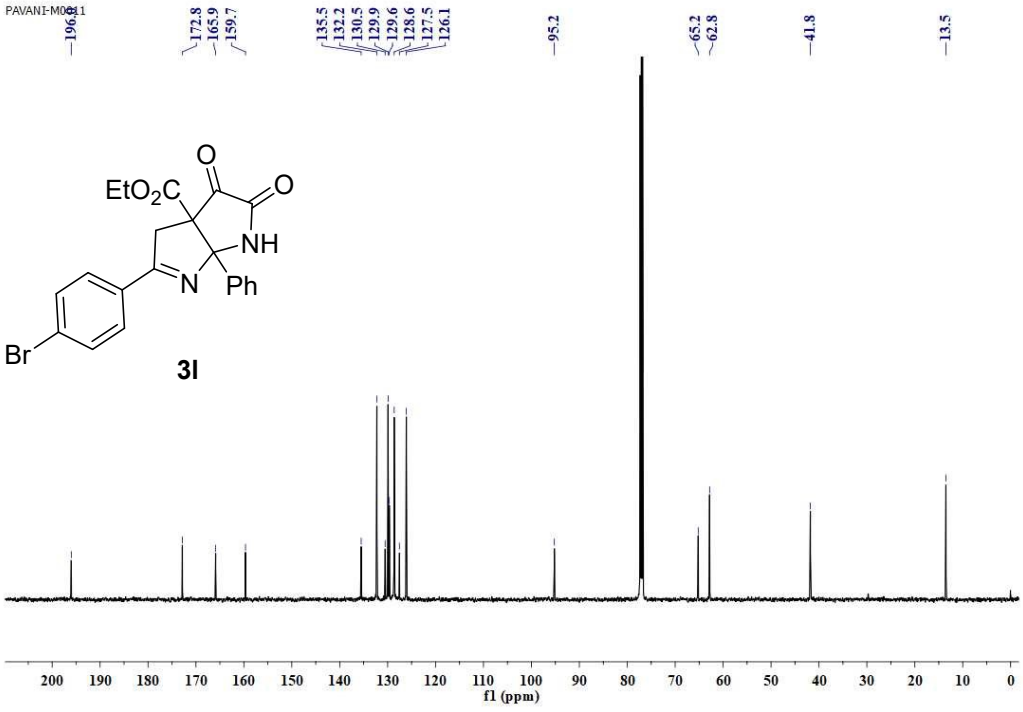
^{1}H-NMR spectrum of **3k** (400 MHz, $CDCl_3$)



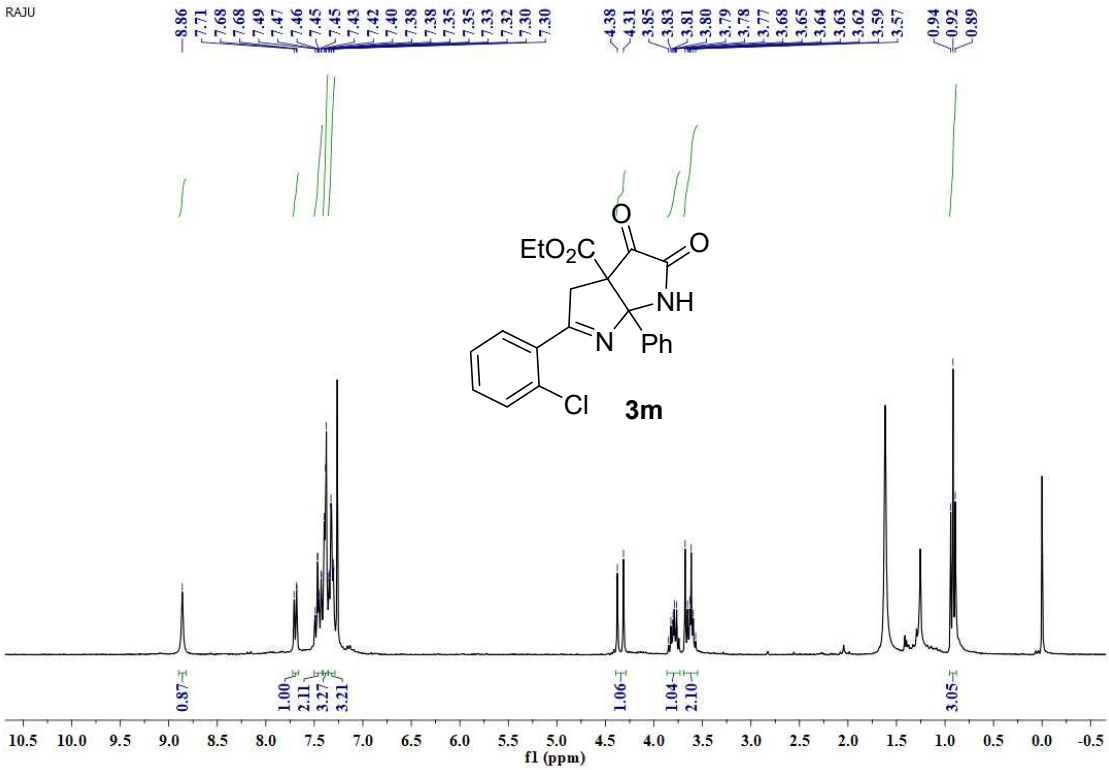
^{13}C-NMR spectrum of **3k** (125 MHz, $CDCl_3$)



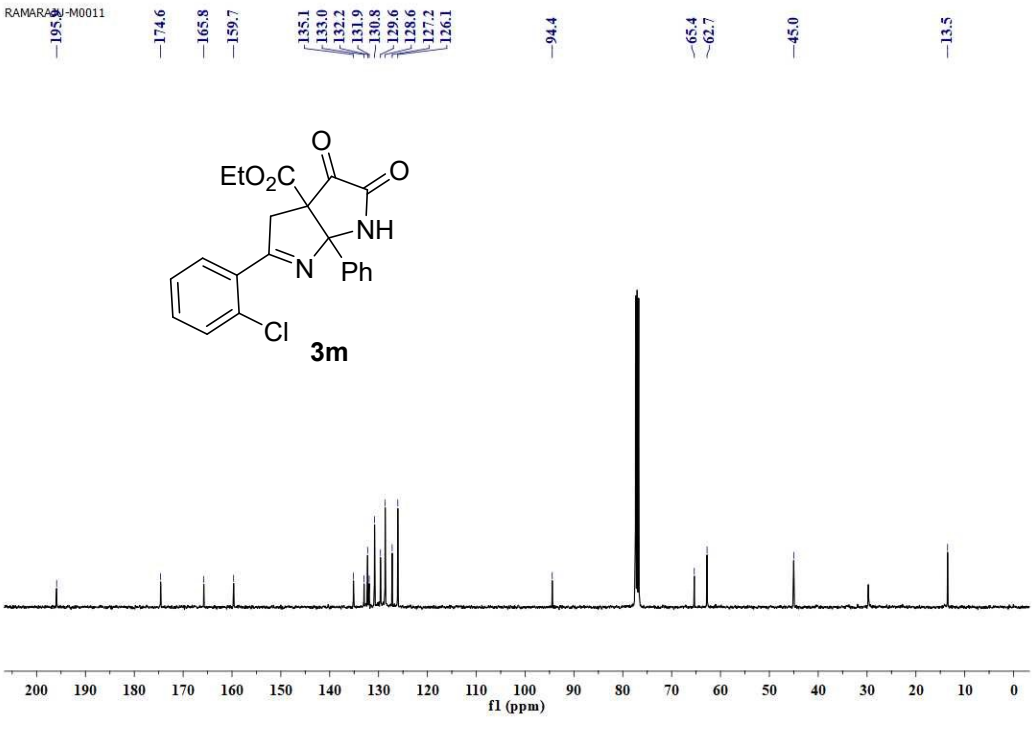
^{1}H-NMR spectrum of **3l** (400 MHz, $CDCl_3$)



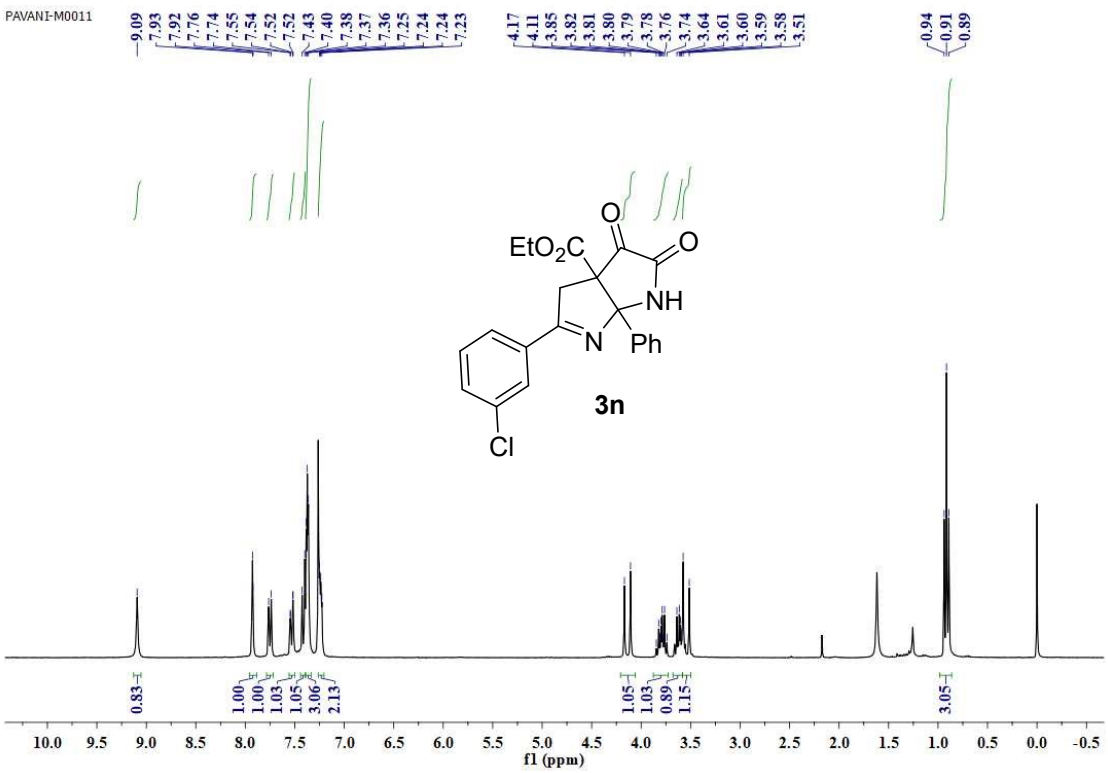
^{13}C-NMR spectrum of **3l** (125 MHz, $CDCl_3$)



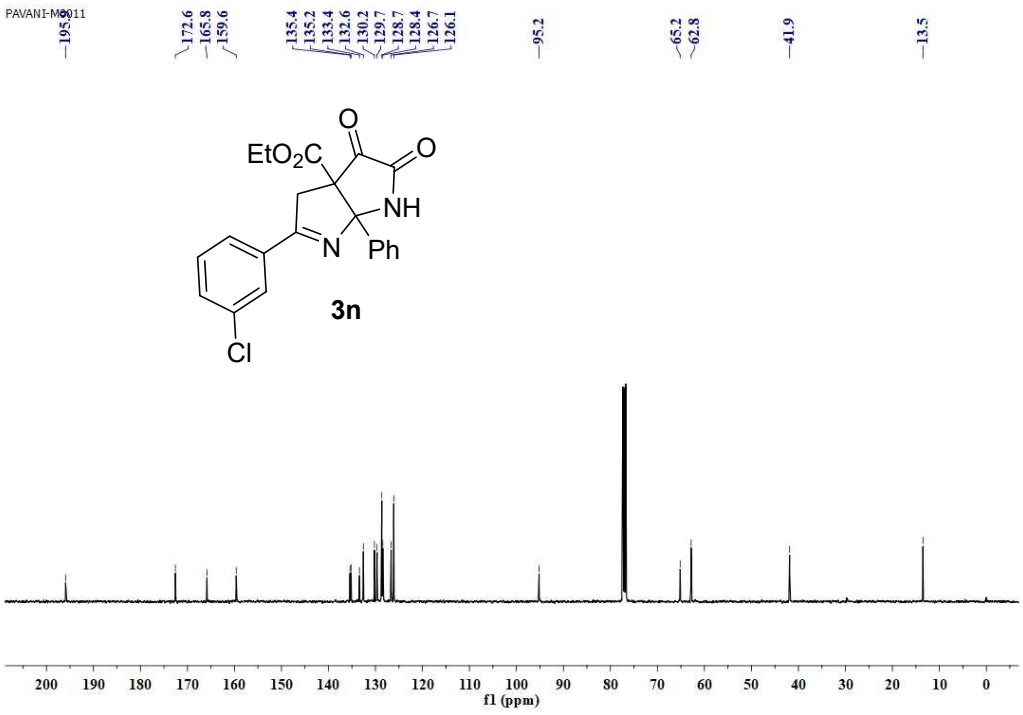
^{1}H-NMR spectrum of **3m** (300 MHz, $CDCl_3$)



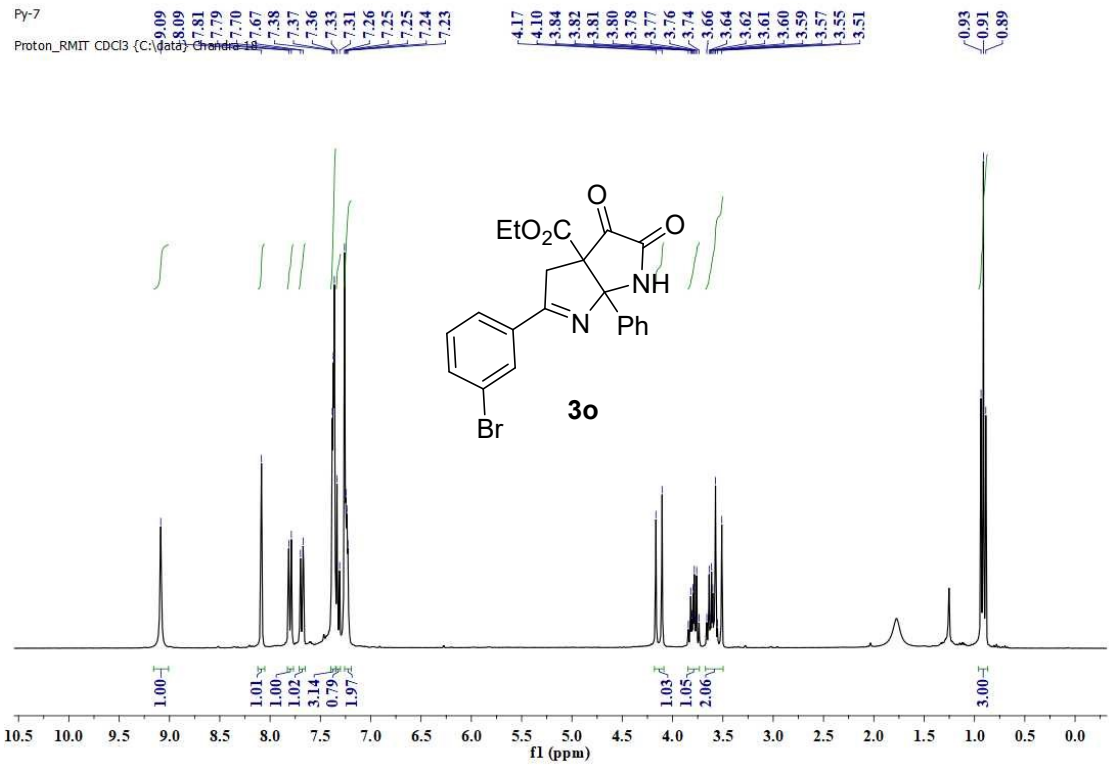
^{13}C-NMR spectrum of **3m** (100 MHz, $CDCl_3$)



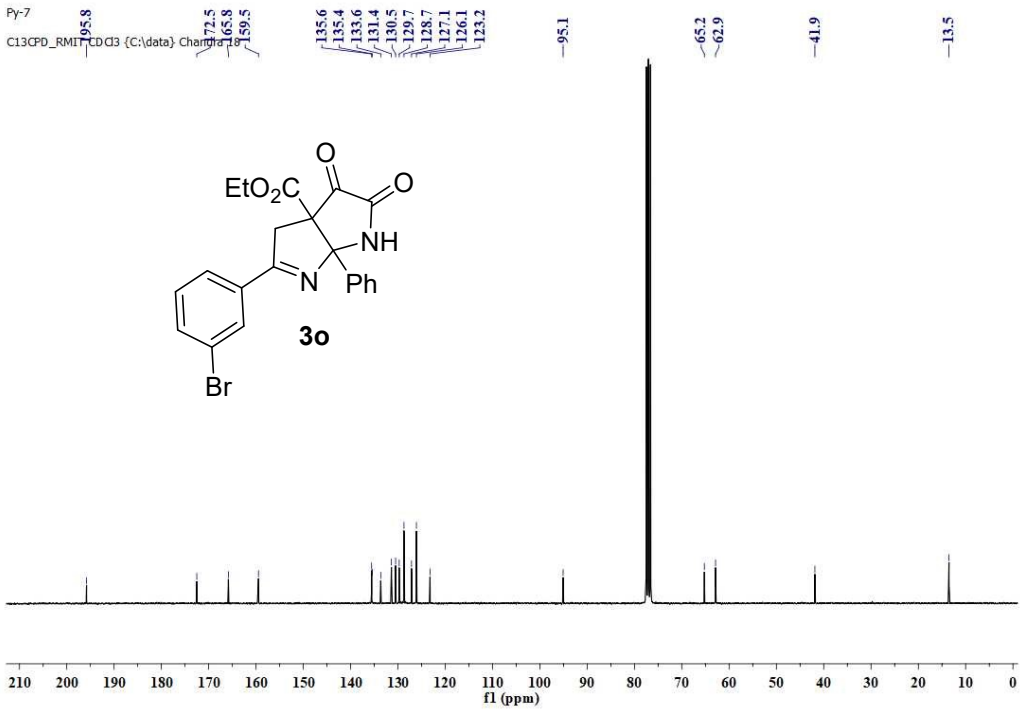
^{1}H-NMR spectrum of **3n** (300 MHz, $CDCl_3$)



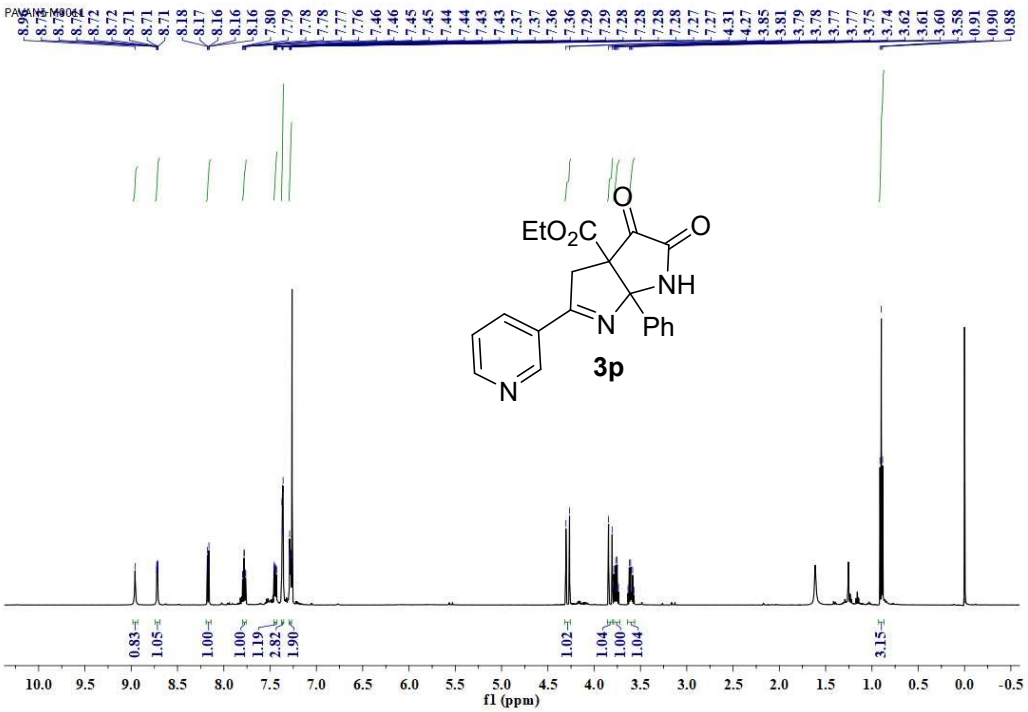
^{13}C-NMR spectrum of **3n** (100 MHz, $CDCl_3$)



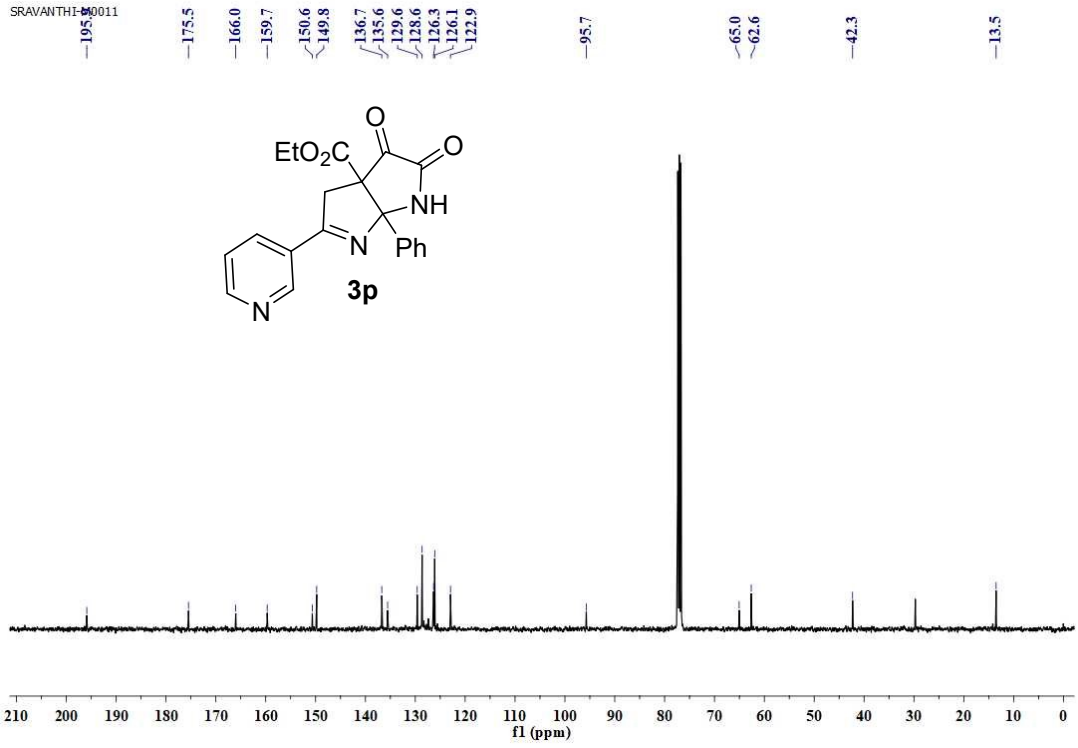
^{1}H-NMR spectrum of **3o** (300 MHz, $CDCl_3$)



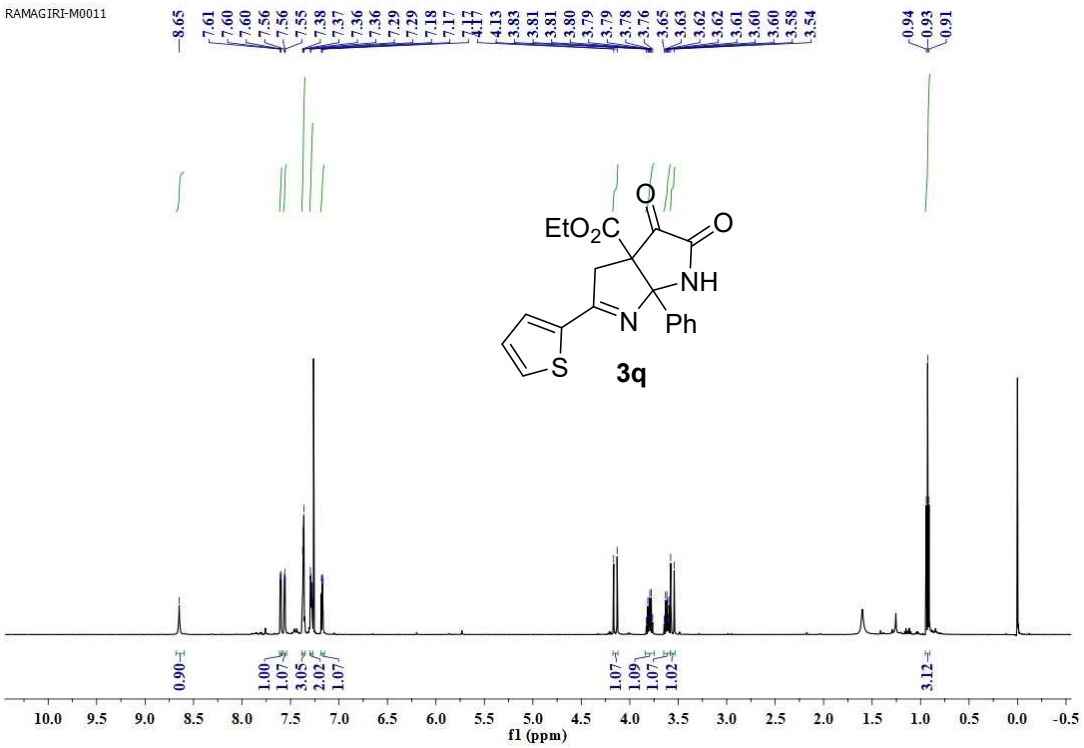
^{13}C-NMR spectrum of **3o** (75 MHz, $CDCl_3$)



^{1}H-NMR spectrum of **3p** (500 MHz, $CDCl_3$)



^{13}C-NMR spectrum of **3p** (100 MHz, $CDCl_3$)



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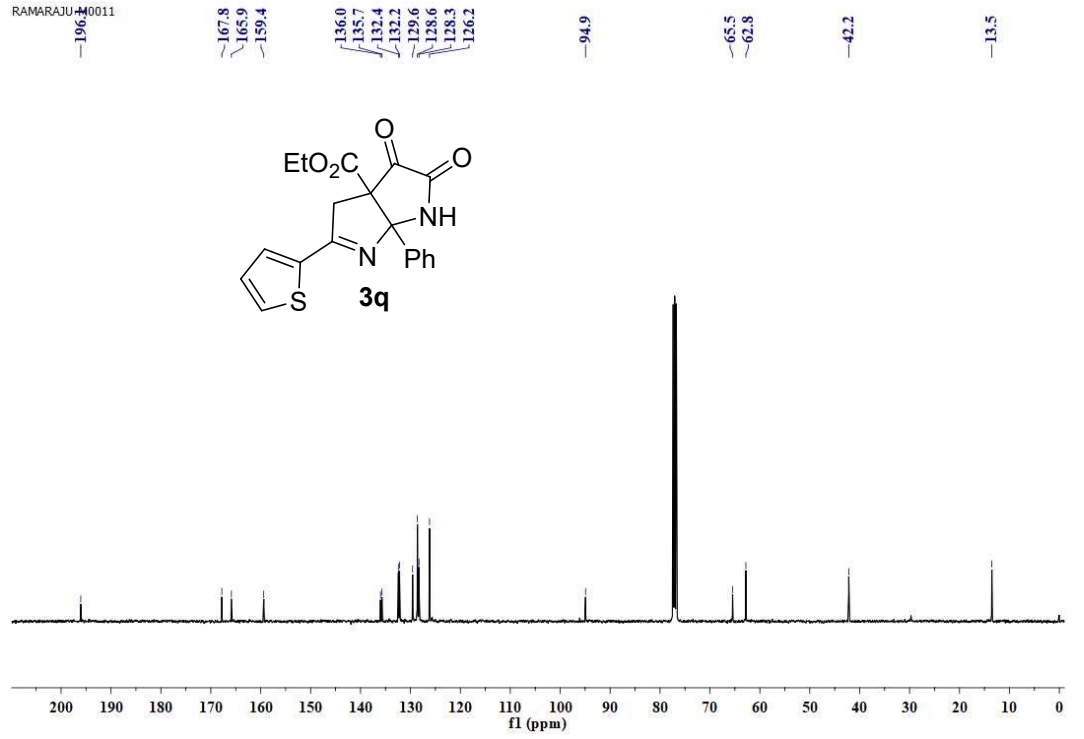
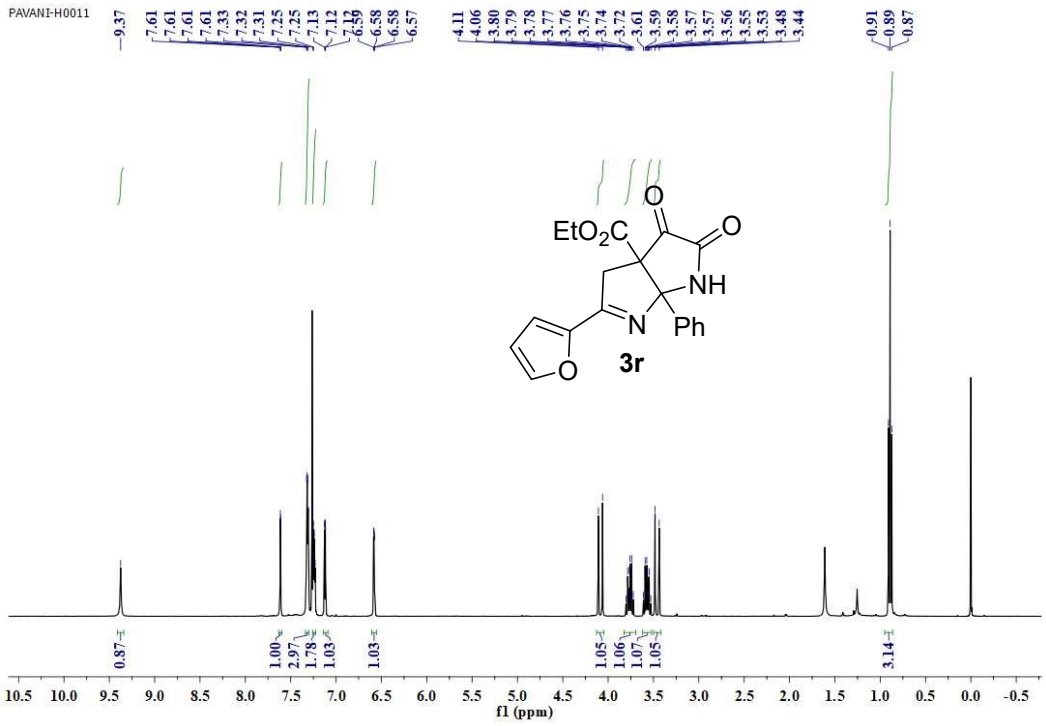
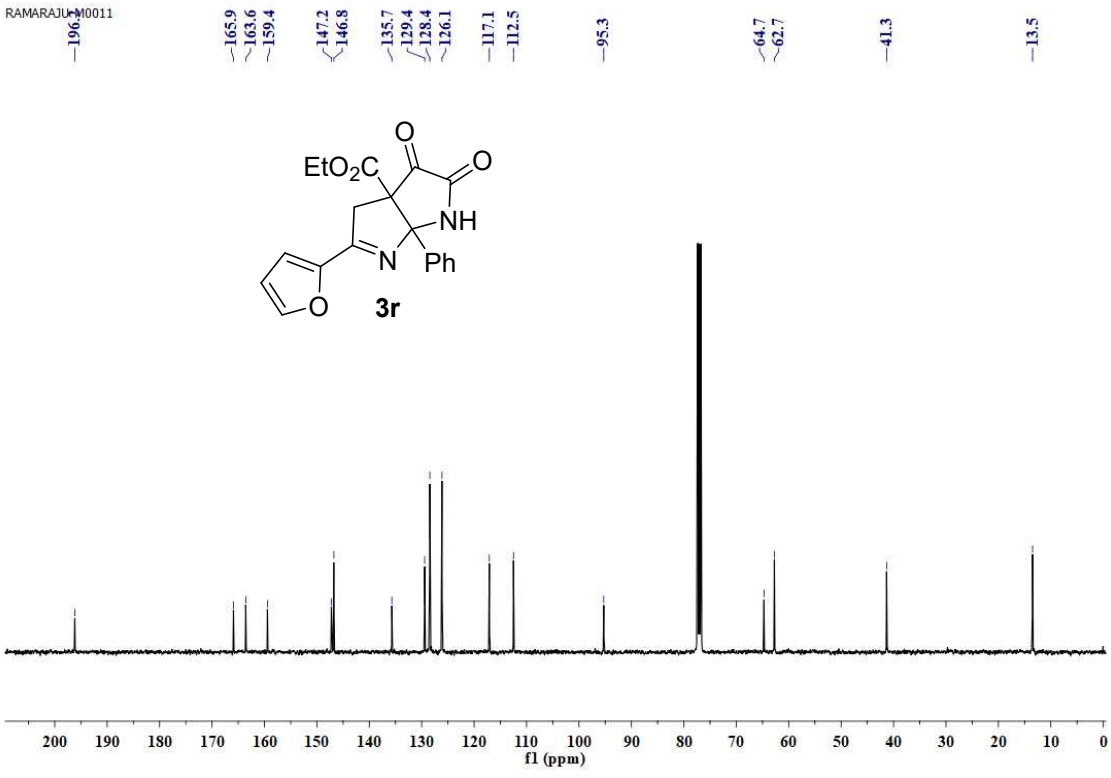


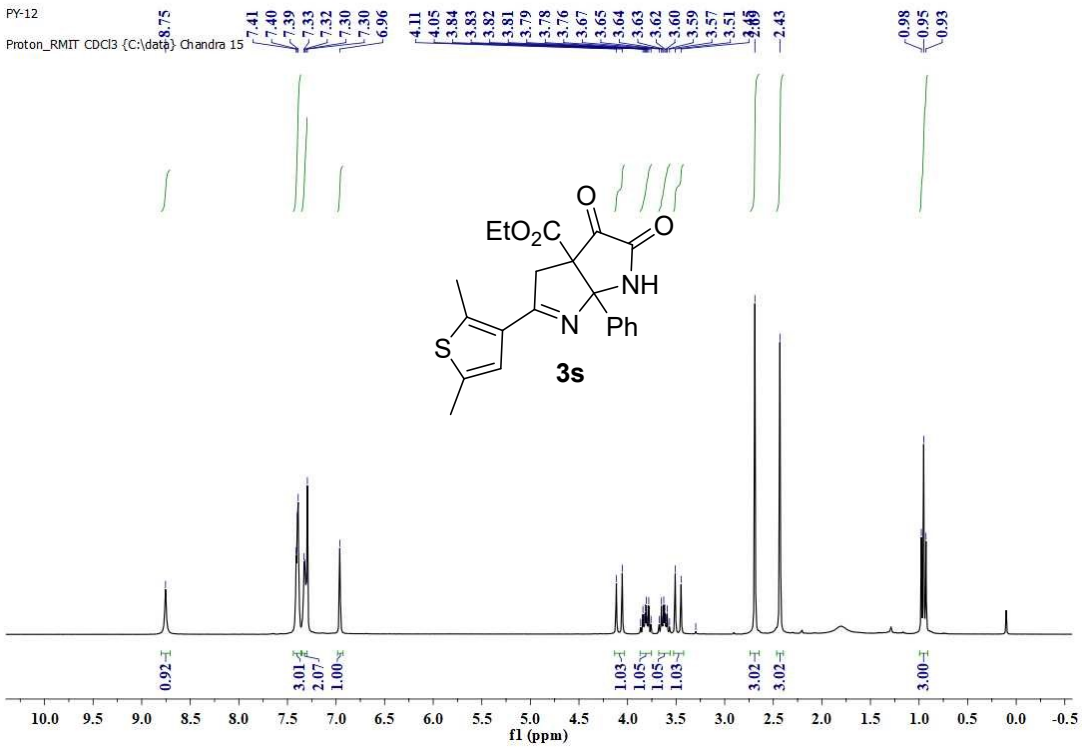
^{13}C-NMR spectrum of **3q** (100 MHz, $CDCl_3$)



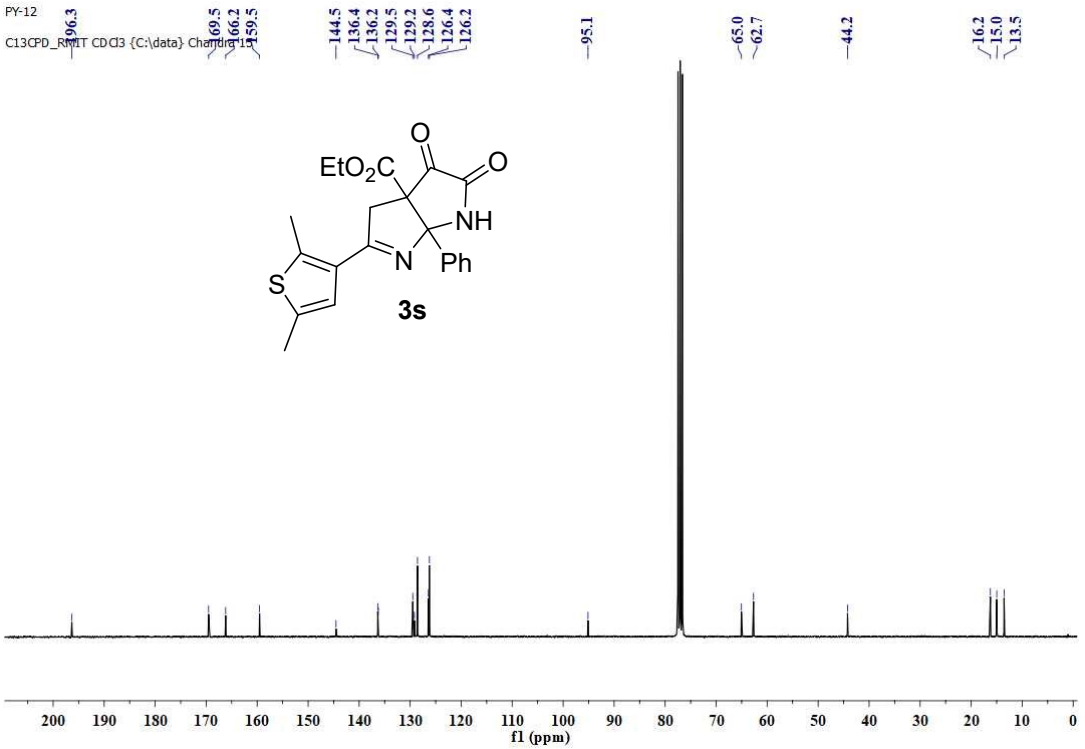
^{1}H-NMR spectrum of **3r** (400 MHz, $CDCl_3$)



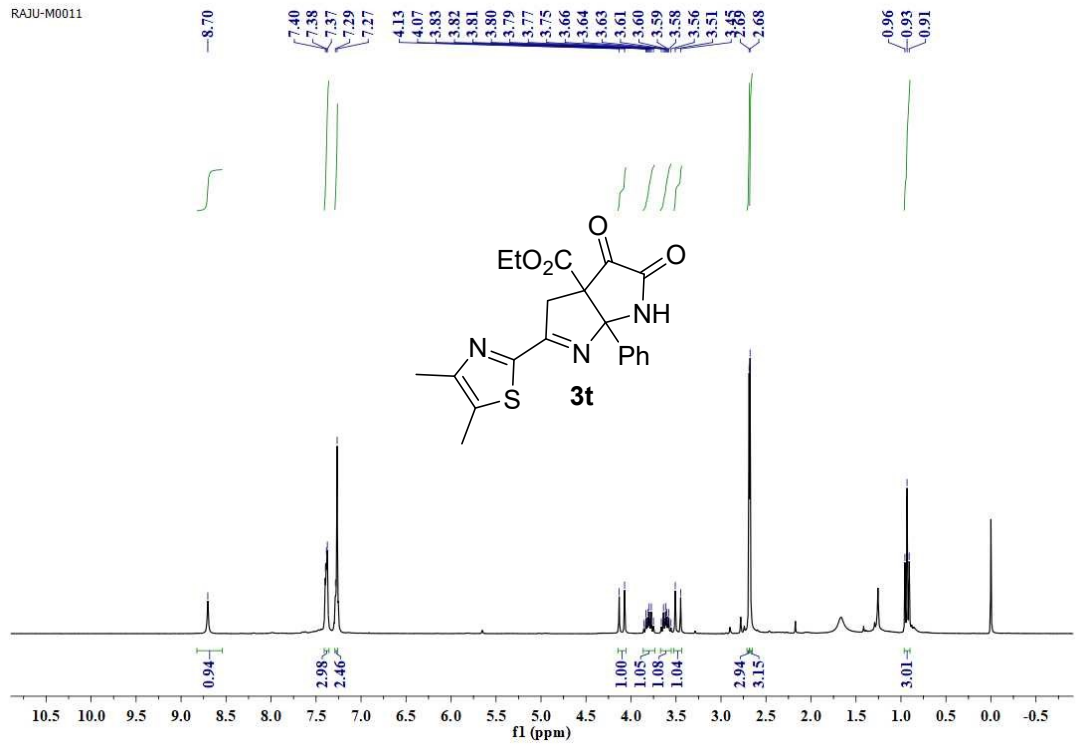
^{13}C-NMR spectrum of **3r** (100 MHz, $CDCl_3$)



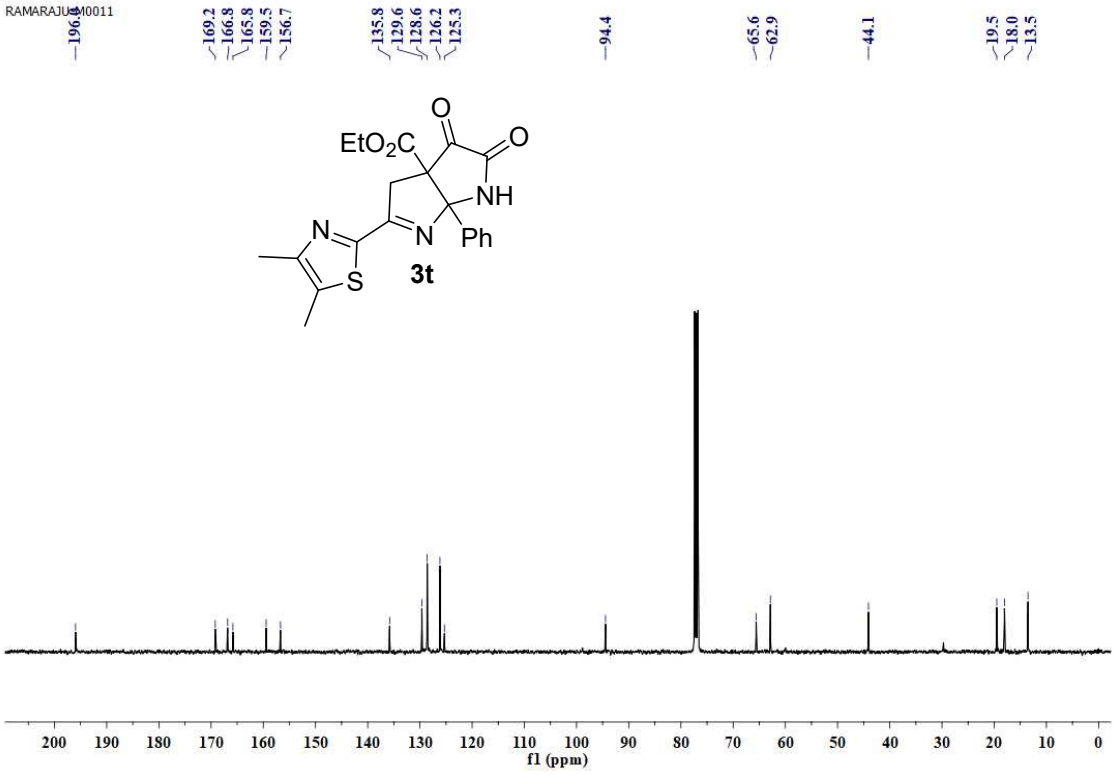
^{1}H-NMR spectrum of **3s** (300 MHz, $CDCl_3$)



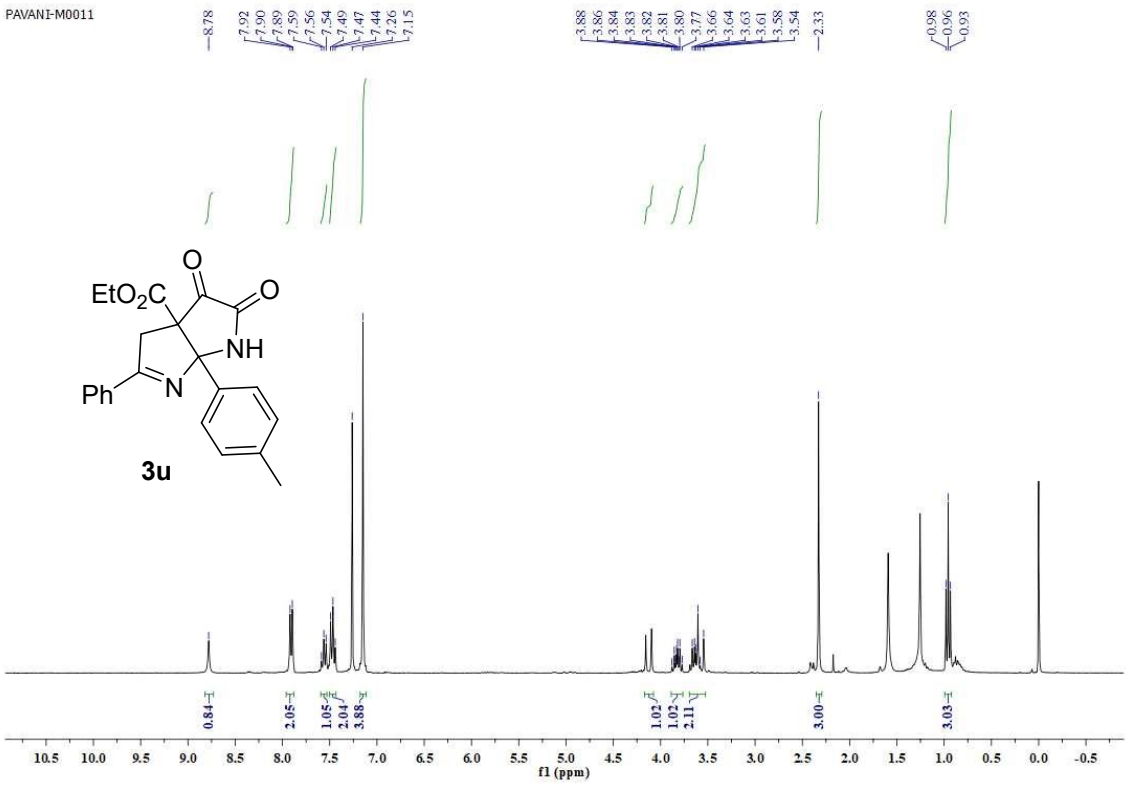
^{13}C-NMR spectrum of **3s** (75 MHz, $CDCl_3$)



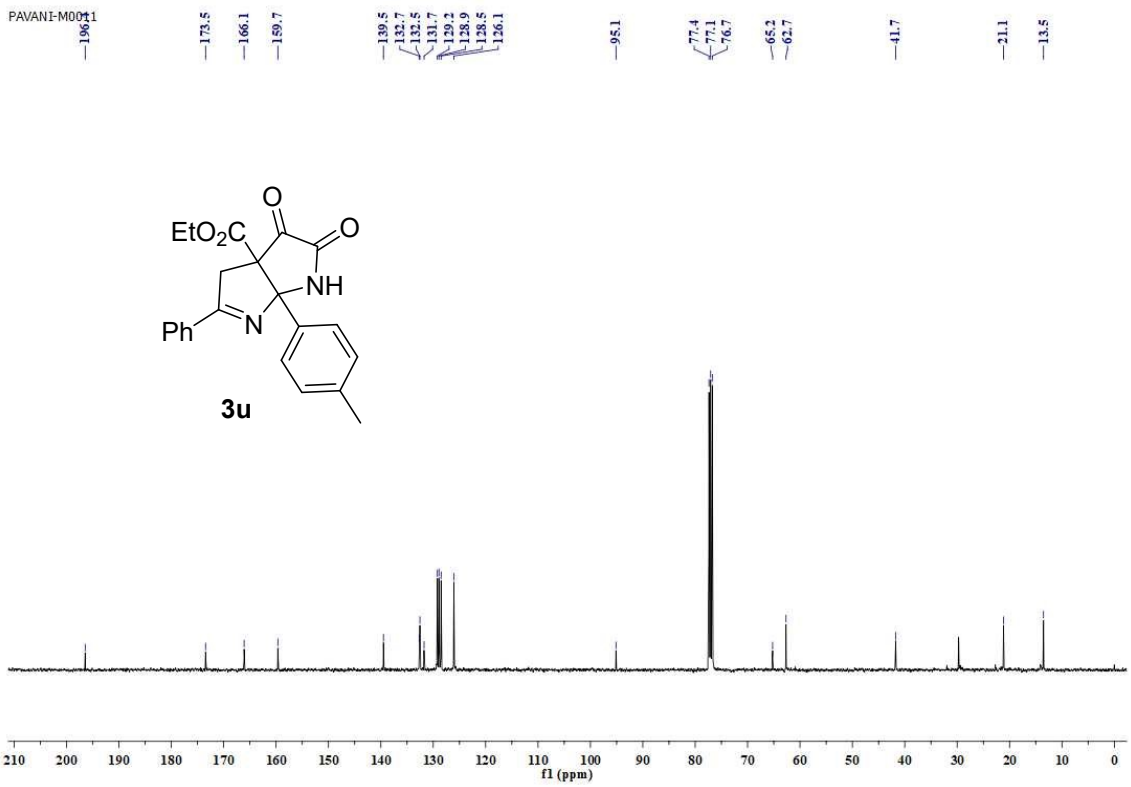
^{1}H-NMR spectrum of **3t** (300 MHz, $CDCl_3$)



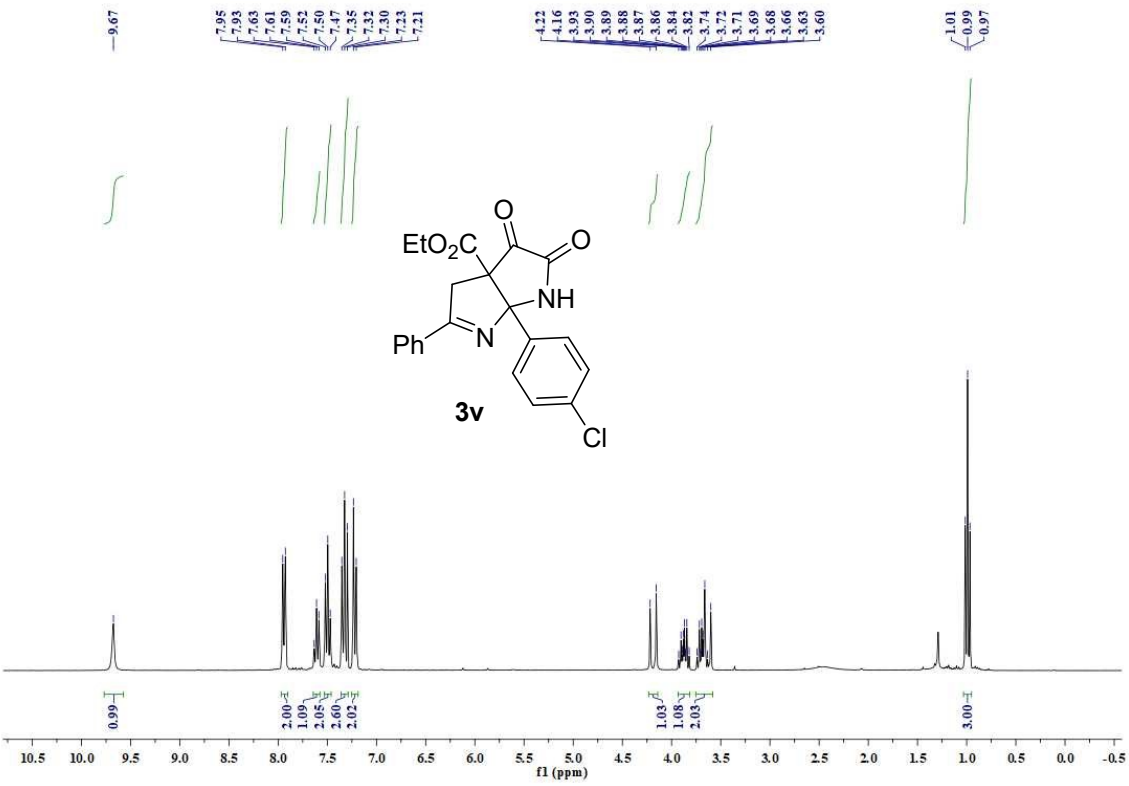
^{13}C-NMR spectrum of **3t** (100 MHz, $CDCl_3$)



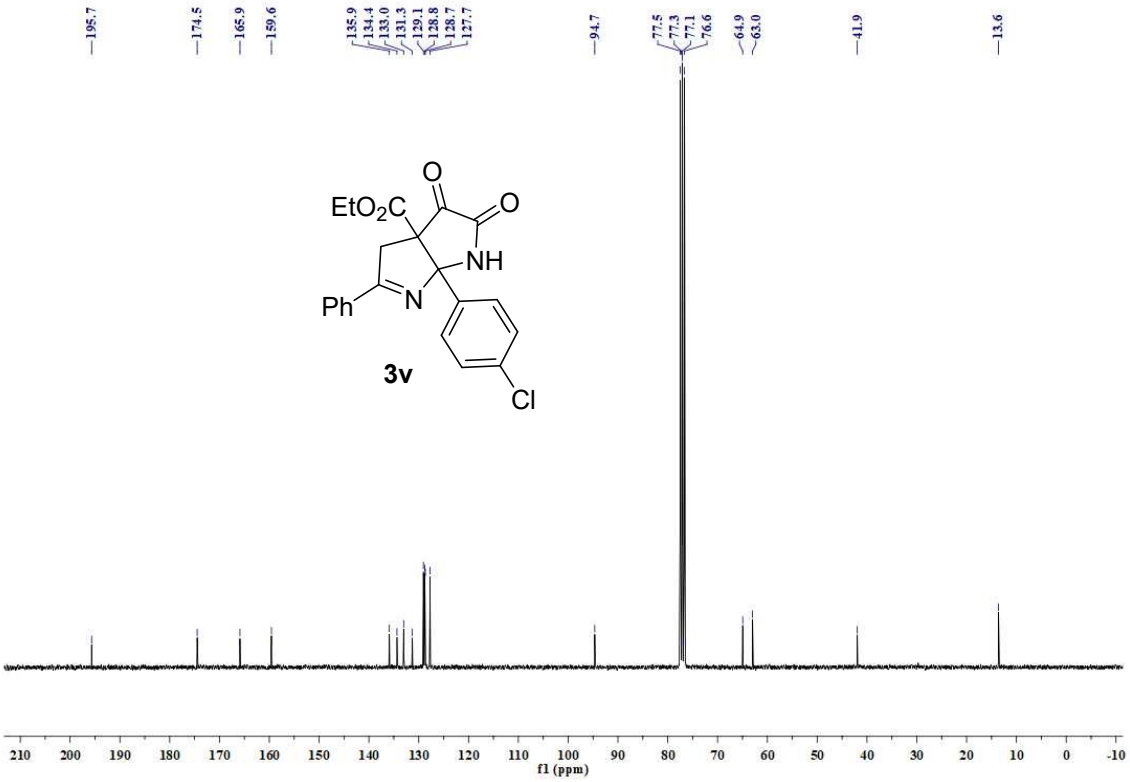
^{1}H-NMR spectrum of **3u** (500 MHz, $CDCl_3$)



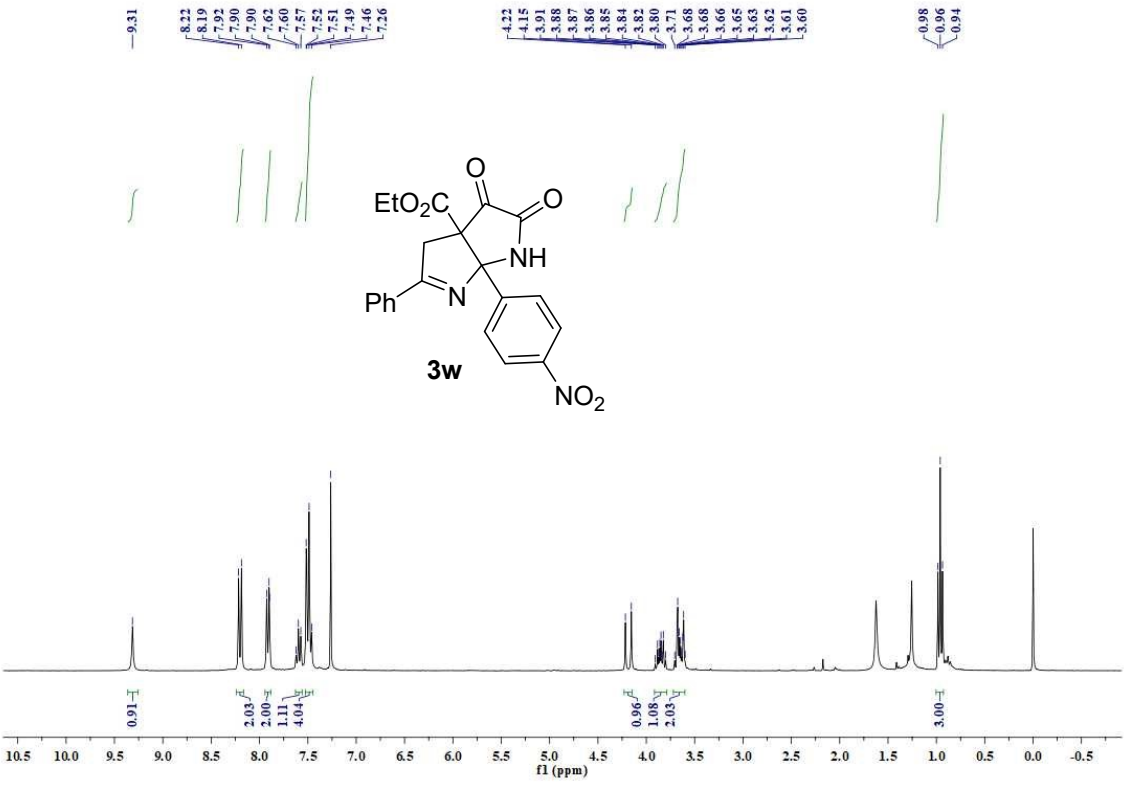
^{13}C-NMR spectrum of **3u** (100 MHz, $CDCl_3$)



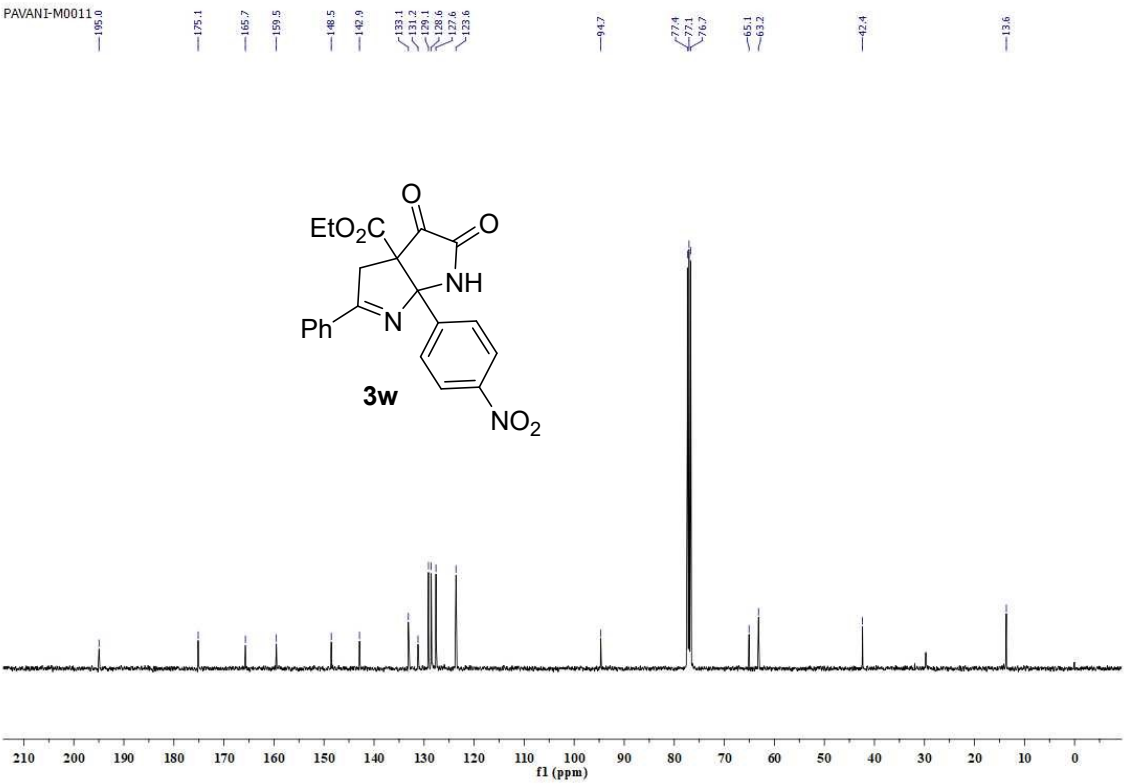
^{1}H-NMR spectrum of **3v** (500 MHz, $CDCl_3$)



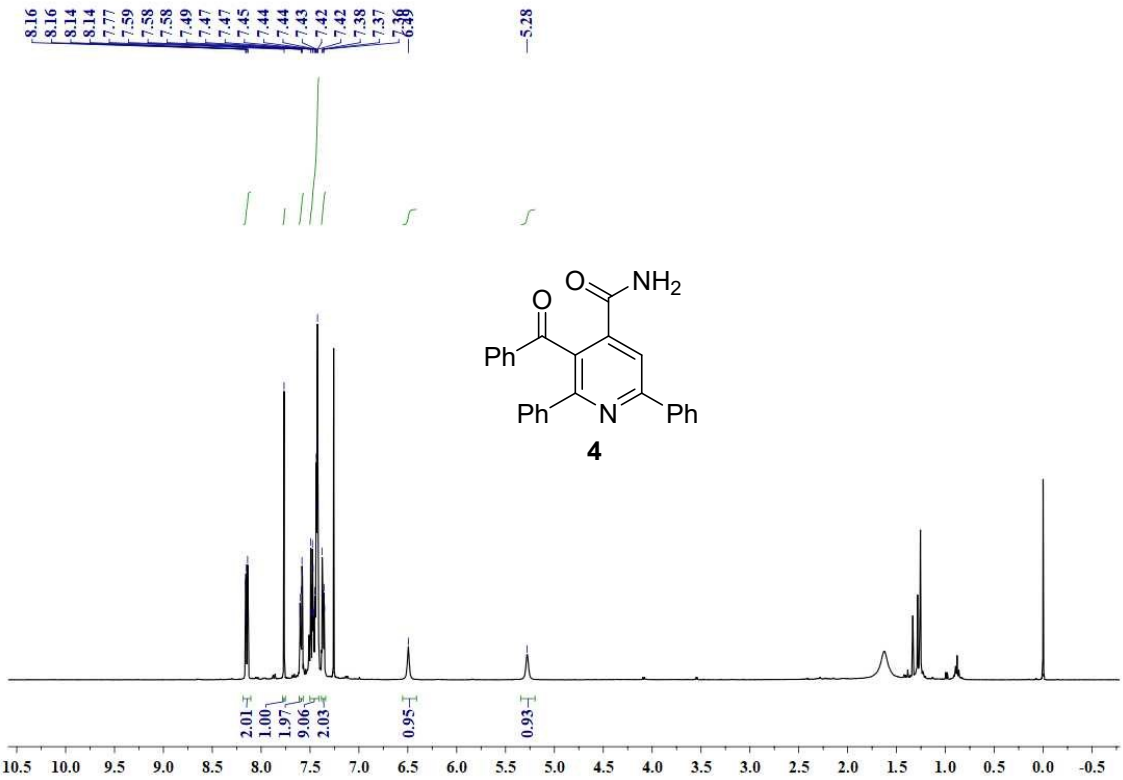
^{13}C-NMR spectrum of **3v** (75 MHz, $CDCl_3$)



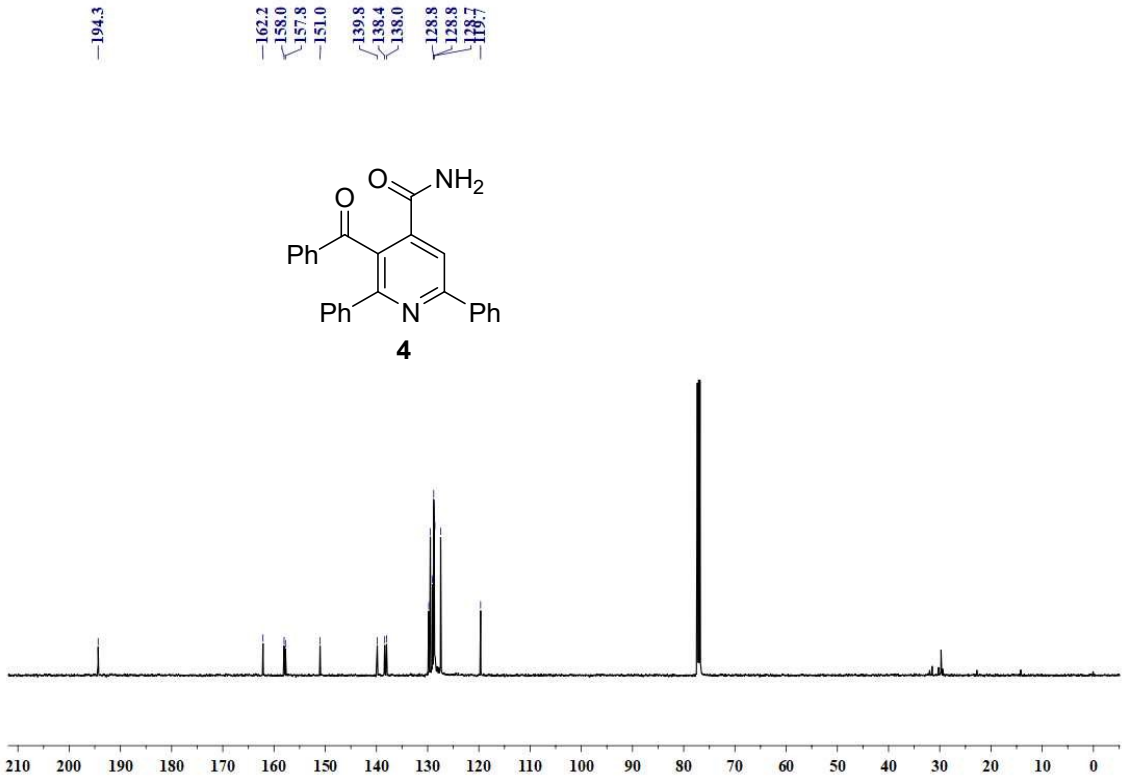
^{1}H-NMR spectrum of **3w** (500 MHz, $CDCl_3$)



^{13}C-NMR spectrum of **3w** (75 MHz, $CDCl_3$)



^{1}H-NMR spectrum of **4** (400 MHz, $CDCl_3$)



^{13}C-NMR spectrum of **4** (75 MHz, $CDCl_3$)